PROSPECTS IN DETERMINISTIC THREE-DIMENSIONAL WHOLE-CORE TRANSPORT CALCULATIONS

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The point we made in this paper is that, although detailed and precise three-dimensional (3D) whole-core transport calculations may be obtained in the future with massively parallel computers, they would have an application to only some of the problems of the nuclear industry, more precisely those regarding multiphysics or for methodology validation or nuclear safety calculations. On the other hand, typical design reactor cycle calculations comprising many one-point core calculations can have very strict constraints in computing time and will not directly benefit from the advances in computations in large scale computers. Consequently, in this paper we review some of the deterministic 3D transport methods which in the very near future may have potential for industrial applications and, even with low-order approximations such as a low resolution in energy, might represent an advantage as compared with present industrial methodology, for which one of the main approximations is due to power reconstruction. These methods comprise the response-matrix method and methods based on the two-dimensional (2D) method of characteristics, such as the fusion method.

KEYWORDS : Transport, Whole-core, 3D, MOC, Fusion Method, Response Matrices

1. INTRODUCTION

These last decades have seen a steady increase in the interest in full transport three-dimensional (3D) calculations for the analysis of reactor cores. This has been accompanied by a continuous increase on modeling and calculations on large-scale parallel computers with thousands of processors. These calculations are intended to eliminate the so-called transport effects in the present diffusion-based calculation scheme. The thesis we advance in this paper is that accurate deterministic core transport calculations are not currently targeted to industry's needs, which require a large number of reactor cycle calculations, sometimes to be performed in relatively short times, comprising many three-dimensional steady-state core calculations. Moreover, one may question the interest of carrying out very expensive and time consuming accurate 3D transport calculations, while other approximations currently used in industrial applications may have a larger or comparable impact on the final results. Finally, regarding deterministic whole-core transport calculations, the emphasis of the developments has been on spatial discretizations and scalability of computations, while not much thought has been given to the generation of

the cross sections needed for such calculations. Questions such as the interest of 3D cross section self shielding calculations or the problem of energy mesh optimization, which is pulled in opposite directions for the need of diminishing the effect of cross section self shielding and that of the increase of anisotropy of scattering due to elastic and inelastic scattering, are still unanswered.

As a justification of our approach these introductory comments are dwelt with in more detail in the first sections of the paper. In the next section we briefly discuss the present status of two-dimensional (2D) assembly and core transport calculations, which have reached industrial maturity, and review some of the codes that perform 3D transport calculations which have potential for application to full core calculations. Section 3 contains our notation for the transport equation and some reference equations for use in the remaining sections. The following three sections deal with the discretizations underlying the deterministic approach to transport. In Section 4 we discuss the universally adopted multigroup energy discretization which, to our knowledge, seems to be the most constraining of the three discretizations. We dwell in particular but briefly with self shielding of resonant cross sections and with the

effect of elastic and inelastic scattering on the anisotropy of multigroup transfers. In the following section we briefly review the PN and SN angular discretizations, while two typical spatial discretizations, the discontinuous finite element (DFE) and the long characteristic (MOC) methods are visited in Section 6. We limit our presentation of the MOC to the familiar case of the step approximation. However, because of the potentiality of the MOC for realistic transport calculations based on higher expansions, we give in Appendix B a presentation of the general MOC equations for a region wise multifunction expansion, as well as an analysis of tracking in large domains.

The following sections contain a survey of present 3D-based transport approximations that we believe have potential for applications in the near future to 3D whole-core deterministic transport calculations meeting industry requirements. Two homogenization-based techniques, much in the spirit of the two-step calculations presently used in the industry, are discussed in Section 8. Both of these techniques aim to eliminate or reduce the errors introduced by the infinite-lattice assembly homogenization technique by including the effect of neighboring assemblies in the homogenization process. The next section discusses interface-current and response-matrix methods. The latter method is based on the pre calculation of assembly response matrices and can be organized as the two-step procedure used by the industry for 3D core calculations with the difference of being fully based on transport, albeit problems remain to be solved for large memory storage and pre computation of the response matrices accounting for burnup. In Section 9 we analyze three numerical techniques based on 2D MOC calculations that allow for approximate or exact 3D transport calculations. Among these, the so-called fusion method has already been recognized as an excellent candidate for one-point steady-state 3D transport calculations. Conclusions are given in the last section.

Part of the material has been relegated to the appendices. Appendix A contains a short description of elastic and level-inelastic scattering. Several technical points and extensions of the MOC are presented in Appendix B. In particular the last section in this appendix contains a description of 3D modular tracking based on assembly typing. Finally Appendix C gives a short description and general formulas for nonlinear coarse mesh acceleration.

The author believes that in the near future realistic whole-core transport calculations for industrial applications would have to be done with a limited number of groups and that, therefore, special care would still have to be put in the preparation of multigroup cross section data and the calculation of their spatial and temporal changes due to temperature and burnup during the reactor cycle. However, given the limited amount of space, the emphasis in this work is on the transport calculation method. Still, even with this limitation in the scope of the paper, some important subjects either have not been discussed at all or, depending on the personal bias and interest of the author, have received

scant attention. In the first group probably the big losers are large scale computation in massively parallel machines and accelerations methods. In particular, no account of the progress, present status and prospects of parallel computations is given, and subjects such as Krylov techniques, preconditioning, parallel architecture, processor communication and scalability, to mention a few, are not discussed. The author recognizes that there will not be true 3D whole-core transport calculations without a heavy dose of parallel computing, but also realizes that there is a continuous stream of publications and conferences on these matters and that he has not much to contribute to this particular subject. Concerning the prospects of applications to reactor physics of large parallel computations, as a starting point the interested reader can consult the proceedings of the workshop on High end computing for nuclear fission science and engineering.⁽¹⁾ Others subjects such as PN and PN-based methods get much less attention than discrete ordinates methods. In Section 6 the description of the discontinuous finite element method is very brief but the author thinks that this subject is abundantly treated in books and in the technical literature. The big winner is the method of characteristics (MOC) and the reason for this is that the method has been proven to be very efficient for two-dimensional transport calculations but, because of its greed for intensive computations and storage requirements, it needs rethinking and complementary research in order to be competitive for large-scale 3D transport calculations.

Finally, a number of individuals have been consulted and have provided advice and help with the contents of this paper but, needless to say, the opinions stated here are the sole responsibilities of the author.

2. GENERAL CONSIDERATIONS

We begin this section with a description of the two-step method used in industrial calculations and with a brief enumeration of the computational methodology and some of the industrial needs concerning reactor calculations. The section ends with an overview of present 2D transport methods utilized by the industry and a review of some of the 3D computer codes that have been developed, but which are mostly used for research in universities and laboratories.

2.1 Present Life

A nuclear reactor is a machine that maintains a nearly steady-state fission chain through a large period of time, typically one year. Therefore, a large part of the analysis needed for the design and follow up of the reactor requires many one-point steady-state core calculations. Moreover, since the temperature distribution is not known at the time of the first core calculation, Doppler broadening for

resonant cross sections has to be done repetitively in an iterative procedure involving neutronic core and thermal-hydraulic calculations.

Today's industry standard for reactor core calculations is based in the well-known two-step procedure where full of piecewise assembly homogenizations based on fine-group lattice transport calculations are used to compile a few-macrogroup parameterized library of homogenized constants, which can then be used for three-dimensional diffusion calculations. This procedure is applied to quasi-static and transient calculations. For reactor cycle analysis the one-point steady-state eigenvalue or source calculation is replaced by multiple one-point steady-state eigenvalue core calculations interlaced with isotopic depletion calculations, which are carried out at consecutive time steps in order to predict, in particular, core power distribution, detailed assembly power distribution, pin peak power value and the cycle length.

A similar depletion calculation done in fine multigroup, two-dimensional transport is applied to each assembly included in the library. Typically, these assembly transport calculations are carried out to a high burnup and require as many as 50 steady-state transport calculations with around 15 time steps per year. These transport calculations are most often done using an infinite lattice model with critical leakage, although other types of reference homogenization problems are also used.⁽²⁾ The assembly burnup calculations have to be repeated for all combinations of the physical parameters that affect the cross sections. Typically, these number three for PWRs: boron concentration, fuel temperature and moderator density.¹ But, with around five different values to be considered per parameter the number of 2D transport calculations can be very large, even though some of the results are obtained by interpolation. Hence, the parameterized library can be very large and, in order to limit its size as well as the amount of transport calculations, usually only 2 or 3 types of assemblies are included in the library. BWRs are characterized by spatial zoning and the large variation of void fraction. For these reactors one has to add two extra parameters, void fraction and void fraction history, and usually include around 6 assembly types in the library. Moreover, at every step the transport calculation has to be repeated with control rods in.

Among others, the integral parameters for which accurate estimates are required comprise the core eigenvalue (k_{eff}), the cycle length and the reactor life span.

The eigenvalue is obtained from a steady-state 3D core calculation. The cycle length results from a constrained optimization of the core loading involving multiple core depletion calculations. The objective of the cycle optimization is to provide as long a cycle as possible while maximizing

the nominal power. Because the latter is limited by fuel integrity, one needs to determine the power distribution and especially the local power peak during the cycle. Presently, the power distribution is obtained using a power reconstruction technique (equivalent to solving an inverse problem with a regularization method.) The resulting error in the power distribution is estimated to be ~2% with fresh fuel and ~6% from irradiated fuel. The latter is because of the increasing uncertainty on material balance which it is estimated to account for the extra 4%. An important result of the cycle analysis is a correct estimate of the material balance. This not only affects the cycle length through production of fissile actinides but it is important for spent fuel storage and recycling. Furthermore, there is also a time bottleneck concerning the calculation of cycle optimization. Because of follow up of network power demand, possible scrams and other incidents affecting power production, it is only at the end of the cycle that the actual power history is known and new cycle optimization and fuel reloading have to be done in the shortest possible time; moreover, the loading machine or a faulty operation can damage an assembly which must be replaced and the optimization of a new loading pattern has to be done in a very short time (one night.)

Finally, the reactor life depends on the vessel irradiation as measured by fast fluence. The latter results from the propagation of neutrons leaving the surface of the core and is best calculated with Monte Carlo. However, the peripheral assembly spectra required for this calculation is usually obtained from simplified 2D or 1D transport calculations which must include a description of the reflector and surrounding materials.

A number of potential scenarios for normal and accidental operation have to be considered for the safety report required for reactor operation. To this end the industry uses a computation methodology with punctual verifications with more sophisticated models. Moreover, experimental and operational feedbacks are used to adjust the results from computations. Examples are the estimation of cycle length, and the use of irradiated fuel analysis to calibrate the error in the estimation of the material balance to ~4%. Other quantities that have to be estimated are the boron efficiency, the critical rod insertion depth, the control rod worth and the moderator and fuel reactivity temperature coefficients.

These can be obtained from the differences between two calculations and are also corrected with measurement during reactor start up. For example, a power map reconstruction at startup with follow up of power build up is used to estimate control rod and boron worth. Another quantity of interest for reactor safety is the reactivity margin at hot 0% power. This is an accident scenario which compounds a main stream break with the most penalizing rod bank withdrawn.

There are two types of biases in the results of the adopted computation methodology. The *methodology*

¹ For specific transient calculations the moderator temperature and density are de-correlated and the number of parameters is four.

bias depends on approximations made for the calculation such as the geometry description, the homogenization processes, the precision on the material balance and the accuracy of the numerical method. In particular, for some problems the 'exact' geometry is not known, this is the case with a material containing a dispersion of a large number of very small components or for the exact position of pebbles in a pebble bed reactor, and a statistical description is then given which may require stochastic homogenization techniques.^{(3),(4)} The *nuclear-data* bias originates on the precision with which these data are known. These two errors affect deterministic as well as Monte Carlo transport calculations, albeit the methodology bias is much more important for the deterministic methods because of the need for discretization in each phase-space variable. Nuclear data are obtained from measurements and from the use of theoretical models which result on estimated averaged values with error bars. Therefore, any 'good' computation method that uses nuclear data should include a means to calculate the impact of the initial uncertainties on the final results, i.e., a technique for uncertainty propagation.

The trend in reactor physics, especially for new concepts such as GEN IV, is to replace experimentation (in particular expensive mock ups) by simulation. This requires a good assessment of the simulation methodology and the reduction of the methodology bias, which can be partially achieved by using 3D transport calculations. Typically, concentrations in the core are computed on average per assembly or for a partition of the assembly but never at the pin level or for the layers in a pin in which different self shielded cross sections have been computed. Hence, Monte Carlo is a reference when the isotopic concentrations are well known but, because of present limitations in computer power and storage, which in particular limit the number of depletion zones, the concentrations are not known in detail after a depletion step and Monte Carlo is not anymore the 'reference'.

2.2 The Experience: 2D Whole-core Transport Calculations

Collision probability techniques and the method of characteristic are presently used by the industry for computation of cross section data from two-dimensional lattice calculations. Because of the large number of calculations required to compile a parameterized library, approximate models based on flux reconstruction are used by the industry.⁽²⁾ The method of long characteristics (MOC) has become a standard for 2D assembly or assembly motifs calculations and can be run with Monte Carlo accuracy with hundreds of groups and thousands of regions with satisfactory computing times.

The MOC is currently applied for 2D whole-core transport calculations and has made its way into industrial computing schemes.⁽²⁾ Table 1 gives a short list of some of the industrial codes that are able to perform 2D core

calculations: CASMO,^{(5),(6)} CRX,⁽⁷⁾ DeCART,⁽⁸⁾ PARAGON⁽⁹⁾ and APOLLO2.^{(10),(2)} Most of the codes based on the MOC use a flat-flux expansion per region. Figure 1 illustrates the region partition for the calculation of a PWR core with 1/8 symmetry while Table 2 shows the advantage of using a higher-order spatial scheme, in this case the surface-linear approximation implemented in the APOLLO2 code.⁽¹¹⁾

2.3 3D 'whole-core' Transport Codes

In the title of this subsection the words whole-core have been set between quotation marks because neither one of the codes so far developed can be used for industrial calculations in the sense discussed in the beginning of the section. Most of these codes have been tested against simplified benchmark problems or simplified reactor problems for one-point steady-state calculations with relatively few groups and with little or no discussion on the actual representativeness of the cross sections data.

Table 1. Some Transport Codes with Capability for 2D Whole-Core Transport Calculations. MOC = Method Of Characteristics, ICM = Interface-Current Method, ST = Step Approximation, CP = Collision Probabilities, LS = Linear Surface Approximation.

Name	Method	Comments
CASMO-4E	MOC	ST
CRX	MOC	ST
DeCART	MOC	ST
PARAGON CP	ICM	CP
APOLLO2	MOC	LS

Fig. 1. Computing Mesh for a PWR Core with 1/8 Symmetry.

This is not to be taken as a negative comment, given that at present time there is not enough computer power to realize a true 3D whole-core transport calculation with enough geometric detail and with realistic physical data which do not introduce unqualified approximations in the calculation.

A number of three-dimensional transport codes have been developed and used for 3D transport calculations. A list of a representative set of these codes is given in Table 3. With the exception of the last two, all the codes in the table can be qualified as ‘exact’ meaning that in theory the numerical discretization used in these codes can be converged to the solution of the three-dimensional

continuous transport equation by refinement of the energy, angle and spatial approximations, with very strong emphasis in the latter. This does not mean, however, that these codes can be actually used to obtain a converged solution of a spatially-detailed whole-core transport calculation because most of them have been designed for transport calculations with homogenized domains at the assembly or pin level, and therefore their use would be prohibitive for detailed pin calculations. Nevertheless, our classification excludes codes based on spatial approximations that cannot converge to the exact continuous solution, such as DeCART⁽¹²⁾ and to less extend COMET.⁽¹³⁾ DeCART is based on the popular ‘fusion’ method⁽¹⁴⁾ which combines two-dimensional MOC and one-dimensional transport calculations to construct accurate solutions for 3D axial reactor cores with no spatial homogenization, while COMET is a response matrix method that uses pre tabulated data computed with the Monte Carlo method² and that is based therefore on the two-step technique. Because these two codes can be considered as excellent candidates for realistic whole-core

Table 2. PWR 900 MWe with 1/8 Symmetry. Step (SC) and Surface-linear (LS) MOC Results Compared to the Monte Carlo Code TRIPOLI4. Quarter-assembly Production Rates Maximum Error and RMS in %. Computing Times are for an AMD Opteron Processor 848 2197 Mhz with 1024 Kb Cache.

MOC	# regions	Δk_{eff} (pcm)	production rates		CPU (S)
			max	RMS	
SC	162949	-245	2.6	1.2	6660
LS	44289	-297	2.9	1.3	3843

² Since this paper is about deterministic transport methods it may seem as an anathema to include this code here. However, the technique behind COMET does not require computing the response matrices with Monte Carlo and, in any case, the choice of using Monte Carlo for this task is excellent for whole-core calculations.

Table 3. Some Transport Codes with Capability for 3D Whole-core Transport Calculations. PN = PN Angular Approximation, SN = Discrete Ordinates Angular Approximation, EP = Second-order Even Parity Equation, FE = Finite Elements, FD = Finite Differences, ST = Step Approximation, SP = Simplified PN, MOSC = Method Of Short Characteristics, MOC = Method Of Characteristics, DFE = Discontinuous Finite Elements, RM = Response Matrix. ANL = Argonne National Laboratory, IC = Imperial College, LANL = Los Alamos National Laboratory, PSU = Pennsylvania State University, CEA = Commissariat à l’Energie Atomique et Aux Energies Alternatives, IPPE = Institute of Physics and Power Engineering, EPM = Ecole Polytechnique de Montréal, KAERI = Korea Atomic Energy Research Institute, GT = Georgia Institute of Technology.

Name	Method	Comments	Origin
VARIANT	PN FE EP	Quadratic	ANL
EVENT	PN FE EP		IC
PARTISN	SN FD	Orthogonal meshes	LANL
PENTRAN TM	SN FD	Cartesian meshes	PSU
IDT	SN MOSC	Cartesian meshes	CEA
MCCA3D	SN MOC	ST	IPPE
DRAGON	SN MOC	ST	EPM
ATTILA [®]	SN DFE	Linear	LANL
MINARET	SN DFE	Axial, Linear	CEA
UNIC	PN & SN FE EP SN MOC	Up to 9th order	ANL
DeCART	SN MOC	Axial, SP ₃	KAERI
COMET	RM	pre tabulated data	GT

transport calculations for industrial applications they will be discussed more in detail in separate sections (Section 8.2 for the response-matrix method and Sec. 9.1 for the fusion method).

Instead of given an exhaustive account of the exact numerical techniques and technical feats behind the codes presented in Table 3 we would limit our explanations to very short comments and address the interested reader to the literature. VARIANT and EVENT are legacy codes based on a finite element approximation of the PN angular form of the second-order even-parity transport equation. VARIANT has been intensively developed during the past years and presently uses a response matrix formulation and techniques to partially decouple lattice from whole core effects by using internal reflective conditions for high order spherical harmonics,^{(15),(16),(17)} while a conjugate gradient technique preconditioned with a nonlinear quasi-diffusion-like tensor is used to solve the PN equations in EVENT.^{(18),(19),(20)}

In the following and unless otherwise indicated all the codes we mention are based on the discrete ordinates (SN) angular approximation of the first-order form of the transport equation. PARTISN and PENTRANTM are based on finite differentiation in orthogonal meshes. PARTISN^{(21),(22)} implements several spatial discretization techniques (diamond, adaptive weighted diamond, linear discontinuous, . . .), allows for adaptive mesh refinement by angular and spatial interpolation and has been optimized to run in massively parallel computers. On the other hand, the parallel code PENTRANTM, while limited to Cartesian meshes, allows for mesh refinement in energy, angle and space and uses an accurate exponential theta-weighted differentiation scheme.^{(23),(24)} IDT is also limited to Cartesian meshes but offers the advantage of implementing the method of short characteristics with up to a bilinear expansion for the volume and surface angular fluxes.^{(25),(26)} MOCCA3D⁽²⁷⁾ and DRAGON⁽²⁸⁾ are based on the method of long characteristics (MOC), whereas ATTILA and MINARET use instead linear discontinuous finite elements, ATTILA⁽²²⁾ and its commercial spin-off ATTILA[®] on unstructured tetrahedral meshes,^{(29),(30)} while MINARET is limited to axial 3D geometries with extruded triangular elements.⁽³¹⁾

Finally, we shall dwell with a bit more of detail on the code UNIC⁽³²⁾ (Ultimate Neutronic Investigation Code) because it has recently been developed with the aim of performing pin-level whole-core transport calculations in massively parallel computers. The code is part of the fast reactor simulation system SHARP and contains three transport solvers: PN2ND, SN2ND and MOCFE. Both, PN2ND and SN2ND, are based on a finite element formulation of the second-order, even-parity form of the transport equation while MOCFE, the most recent development, proposes a MOC solution of the first-order transport equation which uses the finite element mesh generator to mesh the geometry. The PN2ND solver is an

outgrow of the experience acquired in Argonne with the VARIANT code and was intended to provide faster solutions for assembly homogenized cores in massively parallel computers. However it offers a lower spatial approximation because contrarily to VARIANT, which allows for discontinuity of both components of the flux across elements, in PN2ND only the odd angular flux can be discontinuous. The equations of the method are positive definite and the one-group solution is efficiently obtained with a conjugate gradient technique.^{(33),(34)} The SN2ND solver was developed for a better spatial detail with homogenization only at the pin level and was therefore based on the SN angular discretization which, for the same polynomial order, offers a higher degree of spatial accuracy than the PN2ND solver. Both solvers have been applied to the calculation of the homogenized ABTR reactors. As an example of performance, the PN2ND solver took 1.3 hours to run a 33-group, P₉ calculation on 4096 cores.⁽³³⁾ An example of the finite element mesh for the ABTR calculations is shown in Fig. 2. UNIC can use tetragons, prisms and hexahedrons finite elements with polynomial orders up to 9, albeit the numerical results show that higher-order approximations offer little or no advantage. A detailed discussion of the numerical schemes used in UNIC, as well as results for numerous benchmarks using the three flux solvers and analysis of parallel strategies and computation performance, can be found in Ref. (34). Most of the comparisons are usually done on the eigenvalue but in this reference a few comparisons are also given for reaction rates. Another interesting item in this reference is a description of the MC²-3 multigroup cross section generator used for the calculations. UNIC shows excellent weak scalability on up to 163380 cores of BlueGene/P and 131072 cores of CRAY XT5 and was able to perform a SN2ND calculation for the PHENIX EOL benchmark with 33-group, 128 angular directions and $\sim 4 \times 10^6$ vertices in 1900 seconds

Fig. 2. Hexahedron Mesh used for Advanced Burner Test Reactor Benchmark.

(of which nearly half were required for source updating) on 131072 cores of the XT5 machine.⁽³⁵⁾

However, these excellent results are still a far cry from a detailed calculation of a one-point steady-state power reactor, which would require a very large storage for the geometrical mesh and would scale up to a large increase in number of unknowns. Most often, the majority of the codes presented in Table 3 have only been tested against Monte Carlo results in simplified few-group benchmarks^{(36),(37)} or even small and/or simplified homogeneous and heterogeneous reactor models, and most of them reached the limit of their capabilities in averaged or small parallel machines. It has to be pointed out that at present there are more realistic, albeit still simplified, benchmarks for PWR and CANDU reactor cores^{(38),(39),(40),(41)} which can be used as new platform tests for 3D transport codes.

2.4 A remark on Parallel Computers

Today there are a small number of parallel computers with Petaflop capabilities. For example, in the US the so-called ‘class’ machines, with as many as 250000 processors and computing power of the order of 5 Petaflops (requiring a power of ~3 MW), are dedicated to fundamental physics and, with the exception of Blue L, they can be used by anyone under the condition that his application for computer time (a minimum of 4 hours which is equivalent to ~10⁶ CPU time) is accepted; there is the Jaguar machine at Oak Ridge and the Blue A machine in construction at Argonne. At the Idaho National Laboratory (INL) there is a 100% dedicated machine for reactor physics, the ‘fission’ machine, which with 12800 processors can produce 100 Teraflops. There is at least one ‘class’ machine in construction in Europe and, in particular, France has a 50000-processor, 1 Petaflops machine.

With an actual cost of two million dollars the INL ‘fission’ machine could be one of the machines that the industry may adopt in the future, but one may assume on the safe side that desktop computers with 100 to 1000 cores will be available within 10 years for most of reactor physics applications. Because large parallel computers are much expensive to buy and run it may be that in the near future there will not be many of them 100% available for reactor analysis. These machines and intermediary ones, such as the ‘fission’ machine, have already shown the potential for calculations involving a large number of unknowns and have immediate applications to one-point 3D whole-core computations for relatively small of simplified reactor cores and, especially, they show a great interest for novel multiphysics applications such as fuel performance analysis involving neutronics, thermal-hydraulic and structural-mechanics coupled calculations.

Therefore, if research has to have an important impact in the industry, a part of the effort of laboratories and universities should be concentrated in doing better with

average, small scale parallel computers, which in the coming future might be available at low cost and therefore used on a daily basis by the industry.

3. THE TRANSPORT EQUATION

The object of this section is to introduce basic concepts and give reference notation for the transport equation.⁽⁴²⁾ Macroscopic and microscopic cross sections are denoted with Σ and σ , respectively. The transport equation reads

$$\left(\frac{1}{v}\partial_t + L\right)\psi = q + q_0,$$

where v and $E = mv^2/2$ are the neutron speed and energy, $\psi(\mathbf{r}, \mathbf{\Omega}, E)$ is the angular flux, $L = \mathbf{\Omega} \cdot \nabla + \Sigma$ is the transport operator for a purely absorbing medium,

$$q = (\mathcal{H} + \mathcal{F}_\lambda)\psi \quad (1)$$

is the emission density comprising scattering and fission contributions, $\mathcal{F}_\lambda = (1/\lambda)\mathcal{F}$, $\mathcal{H}$ and $\mathcal{F}$ are the scattering and production operators and λ is the eigenvalue.

3.1 Isotropic Media

For reactor calculations the assumption of isotropic media is universally accepted. In this case the isotropic cross sections are independent of the angular direction and the scattering and fission kernels depend only on the initial and final neutron energies and on the cosine of scattering and we can write, for example,

$$(\mathcal{H}\psi)(\mathbf{r}, E, \mathbf{\Omega}) = \int dE' d\mathbf{\Omega}' \Sigma_s(\mathbf{r}, E' \rightarrow E, \mathbf{\Omega}' \cdot \mathbf{\Omega}) \psi(\mathbf{r}, E', \mathbf{\Omega}').$$

It is then customary to expand the scattering contribution into spherical harmonics

$$(\mathcal{H}\psi)(\mathbf{r}, E, \mathbf{\Omega}) = \sum_m A_m(\mathbf{\Omega}) \int dE' \Sigma_m(\mathbf{r}, E' \rightarrow E) \Phi_m(\mathbf{r}, E'), \quad (2)$$

where the $A_m(\mathbf{\Omega})$ are real spherical harmonics,³ $m = (k, l)$ is a double index with $k \geq 0$ and $-k \leq l \leq k$ and the

$$\Phi_m(\mathbf{r}, E) = \int_{(4\pi)} d\mathbf{\Omega} A_m(\mathbf{\Omega}) \psi(\mathbf{r}, E, \mathbf{\Omega})$$

are the angular flux moments. We note that the angular moment of the transfer kernel,

$$\sigma_m(E' \rightarrow E) = \frac{1}{2} \int_{-1}^1 d\mu \sigma_s(E' \rightarrow E, \mu) P_{k(m)}(\mu),$$

depends only on the first spherical harmonic index k . Also, in practical applications the sum in m in (2) is done for a finite degree of anisotropy K so that $0 \leq k(m) \leq K$.

³ For details see Ref. (43). The real spherical harmonics obey similar relations to those of the complex spherical harmonics: $\int d\mathbf{\Omega} A_m(\mathbf{\Omega}) A_{m'}(\mathbf{\Omega}) = 4\pi \delta_{mm'}$, $(2k+1)P_k(\mathbf{\Omega} \cdot \mathbf{\Omega}') = \sum_l A_{kl}(\mathbf{\Omega}) A_{kl}(\mathbf{\Omega}')$.

Finally, for the neutron fission source one makes the assumption that fission is isotropic and that the fission spectrum does not depend on the energy of the neutron causing fission, so that the kernel of the production operator is of the form

$$(v\sigma_f)(E' \rightarrow E, \mathbf{\Omega}' \cdot \mathbf{\Omega}) \sim (v\sigma_f)(E') \frac{1}{4\pi} \chi(E)$$

with $\int dE \chi(E) = 1$. However the fission spectrum depends on the type of fissile or fissionable isotope and we have to write

$$(\mathcal{F}\psi)(\mathbf{r}, E, \mathbf{\Omega}) = \frac{1}{4\pi} \sum_x \chi_x(E) \int dE' (v\Sigma_f)_x(\mathbf{r}, E') \Phi(\mathbf{r}, E'),$$

where the sum is over the fissile and fissionable isotopes around position $\mathbf{r}$ and $\Phi = \Phi_0$ is the scalar flux.

3.2 Boundary Conditions

A unique solution of the transport equation is fully defined by the volume sources and the initial and boundary conditions. The latter consist on specifying the angular fluxes entering the domain. To discuss boundary conditions we note ψ_{in} and ψ_{out} the fluxes entering and exiting the domain. The boundary condition can be a fixed entering angular flux or, for reentering conditions, may be defined by a rule which allows to compute the entering flux in terms of one or more exiting fluxes. This rule can be a one-to-one relation between a part of the exiting boundary and a part of the entering boundary, $\pi : (\mathbf{r}_{out}, \mathbf{\Omega}_{out}) \rightarrow (\mathbf{r}_{in}, \mathbf{\Omega}_{in})$, and we shall denote the part of the boundary where this rule applies as the closed component of the boundary. Examples of *closed* boundary conditions are geometric motions or symmetries such as translations, rotations and specular reflections.⁴ The remaining part of the boundary will be called the *open* component. This component comprises the part of the boundary where the mapping π is not one-to-one, as well as the part of the boundary where one has an inhomogeneous boundary condition of the form $\psi_{in} = \psi_0$, where ψ_0 is a fixed angular flux. Examples of open boundary conditions are vacuum and albedo boundary conditions.

3.3 Typical Transport Problems in Reactor Analysis

For time-dependent calculations the eigenvalue λ is set to 1. For steady-state calculations the external source q_0 can be present, for example for source-driven reactors, in which case λ is also set to 1, but for typical core calculations the external source is set to 0 and the steady-state equation becomes an eigenvalue problem

$$(\mathbf{\Omega} \cdot \nabla + \Sigma)\psi = q \quad (3)$$

with q as in Eq. (1).

⁴ Or refraction for photon transport.

Basically, there are two types of time-dependent calculations that are considered for industrial calculations. Kinetic calculations are used in the analysis of safety issues, such as accident scenarios, and are characterized by large changes in reactivity. In these conditions the flux changes in a very fast time scale and the equation has to be solved via a discretization in time with a very small time step. The kinetic transport equation is coupled with the equations describing the evolution in time of precursor concentrations and the external source q_0 contains the delayed-neutron contribution and, in exceptional conditions such as reactor startup, an extraneous source.

The second type of problem concerns reactor design and operation and consists of analyzing the functioning of the reactor at nominal power during the reactor cycle. The assumption here is that, except for small fluctuations, the flux remains constant in time. This translates into the so-called quasi-static approximation according to which $\partial_t \psi \sim 0$. However, the change in isotopic concentrations has to be included in the picture and the transport equation to be considered is the steady-state eigenvalue equation with time-dependent cross sections. This equation is coupled to the Bateman equations describing isotopic depletion. Finally, a supplementary approximation, based on the assumption that the transport flux changes very slowly as the isotopic concentrations change with burnup, allows to decouple the transport calculation proper from the isotopic depletion step. Thus, the final cycle calculation is done by performing a number of steady-state eigenvalue flux calculations at increasing times throughout the cycle, $t_0 < t_1 < \dots < t_N$, while updating the isotopic concentrations from one time to the next by integrating the isotopic depletion equations in time. When possible the updating is done using the previous history to extrapolate the reaction rates and fluxes needed to solve the Bateman equations and, when necessary, by reducing the time interval when the variations are large.

3.4 Transport along a Trajectory

All deterministic methods for the solution of the transport equation, and especially those based on the discrete ordinates form, are based on the spatial discretization of the ballistic form of the equation, i.e., the transport equation for neutrons moving along straight trajectories through a purely absorbing medium. Because $\mathbf{\Omega} \cdot \nabla$ is the directional derivative along the trajectory one can set $\mathbf{r} = \mathbf{r}_\perp + x\mathbf{\Omega}$, where $\mathbf{r}_\perp$ is a two-dimensional coordinate on a plane orthogonal to the direction or propagation $\mathbf{\Omega}$ and x is the coordinate along the trajectory, so that $\mathbf{\Omega} \cdot \nabla \rightarrow \partial_x$. Moreover, since $\mathbf{r}_\perp$, E and $\mathbf{\Omega}$ are constant along the trajectory, all variables and functions can be written as functions of x and the stationary transport balance equation (3) reads

$$(\partial_x + \Sigma)\psi = q, \quad (4)$$

where $\Sigma(x) = \Sigma(\mathbf{r}_\perp + x\mathbf{\Omega}, E)$, $\psi(x) = \psi(\mathbf{r}_\perp + x\mathbf{\Omega}, E, \mathbf{\Omega})$ and $q(x) = q(\mathbf{r}_\perp + x\mathbf{\Omega}, E, \mathbf{\Omega})$. By solving this equation for $\psi(x)$

one obtains the integral form of the transport equation:

$$\psi(x) = e^{-\tau(x)}[\psi_- + \int_0^x dy e^{\tau(y)} q(y)], \quad (5)$$

where ψ_- is the angular flux at position $x = 0$ along the trajectory and $\tau(x) = \int_0^x dy \Sigma(y)$ is the optical distance from $x = 0$ to x . For later use we write this equation for a trajectory crossing a homogeneous region of total cross section Σ :

$$\psi(x) = e^{-\Sigma x}[\psi_- + \int_0^x dy e^{\Sigma y} q(y)]. \quad (6)$$

4. ENERGY DISCRETIZATION

The multigroup form of the continuous-energy transport equation (CETE) is derived by a process of homogenization where energy-dependent cross sections and transfer kernels are replaced by representative group constants. Although for reactor applications one may assume that the medium is isotropic, it is well known that a homogenization process based on preservation of group-averaged reaction rates results in a multigroup equation in an anisotropic medium. More specifically, the multigroup total cross sections become angle dependent, $\sigma(E) \rightarrow \sigma^g(\mathbf{r}, \mathbf{\Omega})$, and the anisotropic components of the transfer kernel include a dependence on the second index of anisotropy, $\sigma_{k(m)}(E) \rightarrow \sigma_m^g(\mathbf{r})$. For details on this homogenization process see Ref. (42) and also Section 7.2.

However, the premises on which this homogenization is based are not realistic because the reaction rates from the solution of the CETE are not known, and the way out of this dilemma is to consider groups that are thin enough so the variation of the cross section within the group is very small and one can write $\tau^g = \int_g dE \sigma(E) \psi(\mathbf{r}, \mathbf{\Omega}, E) = (\sigma^g + \epsilon) \psi^g$, where σ^g is the group-averaged value of $\sigma(E)$, $\psi^g(\mathbf{r}, \mathbf{\Omega}) = \int_g dE \psi(\mathbf{r}, \mathbf{\Omega}, E)$ is the group-integrated angular flux and $\epsilon \ll \sigma^g$ is a small correction term. In these conditions one can introduce an energy-dependent weight function to account to first order for the small correction term and write

$$\sigma^g(\mathbf{r}, \mathbf{\Omega}) = \frac{\tau^g}{\psi^g} \sim \sigma^g = \frac{\int_g dE \sigma(E) w(E)}{\int_g dE w(E)}, \quad (7)$$

where the weight function $w(E)$ is typically an infinite-medium approximation representative of the spectrum of the core (or of a spatial subdomain of interest) being considered. A similar approximation is also made for the transfer kernel.

4.1 Multigroup Self Shielded Cross Sections

The assumptions under which approximation (7) is valid are not realistic for cross sections that change very fast with energy, such as those for resonant isotopes in their resonance range, because this would lead to a very large number of groups (of the order of 40000 or more

for thermal reactors). For realistic multigroup transport calculations it is thus necessary to introduce another homogenization technique, i.e., a method to compute multigroup self shielded cross sections, whereby group-averaged cross sections for resonant isotopes are computed by preservation of group-averaged reaction rates,

$$\sigma^g(\mathbf{r}) \sim \frac{\int_g dE \sigma(E) \Phi(\mathbf{r}, E)}{\int_g dE \Phi(\mathbf{r}, E)},$$

where $\Phi(\mathbf{r}, E)$ is the scalar flux solution of a *reference model problem* representative of the spectrum around location $\mathbf{r}$.

Although the resolution of space and temperature dependent resonance self-shielding is essential in practical power reactor calculations, a detailed account of multigroup cross section self shielding methods is out of the scope of the present work and here we shall give only a brief overview of the technique.

Depending on the type of reactor, two general methods are used. The sub-group method, used for fast reactors where resonance self shielding is significant in the unresolved range, is based on the assumptions that on each group a) the neutron source and the cross sections are uncorrelated and b) the cross sections of a resonant isotopic mixture are uncorrelated. The first assumption allows taking the model problem equal to the actual problem to be solved, leading to an iterative computation of the multigroup self shielded cross sections during the external iterations, while the second assumption simplifies the calculation of mixture resonant effects.

The subgroup assumption is not possible for thermal reactors, which are characterized by a strong absorption in the resolved range. For these reactors one is brought to introduce a simplified reference model problem, typically a model representing slowing down in the resonance range for the problem entire domain or, most often, for smaller subdomains or even for artificial local problems surrounded by a buffer. Moreover, a simplified slowing-down resonance model (narrow, wide or intermediary resonance approximations, or even a version of the subgroup approximation) is then introduced and the solution of the resulting simplified problem is used to obtain an equivalent background cross section. Finally, this cross section is employed to get reaction rates from pre tabulated values, which have been computed in an infinite homogeneous medium with ultra fine multigroup calculations. Because the reference model problem is different from the actual problem to be solved, often an equivalence step is introduced to obtain the final multigroup self shielded cross sections. Sophisticated self shielding techniques describing the detailed rim effect throughout depletion as well as accounting for detailed resonance interference effects⁽²⁾ can have a significant impact on computing time. Thus, today's tendency for 2D transport calculations is to increase the number of groups and use simpler techniques, together with simplified 1D reference model problems,

so as to lessen the impact of the self shielding on the final results as well as to reduce the overhead resulting from the self shielding computation. To our knowledge the need for 3D computations of multigroup self shielded cross sections has not been analyzed yet, but this analysis could possibly be done with Monte Carlo. An application of the collision probability method in RZ geometry to the self shielding of gray Gadolinia fuel pin absorbers in BWRs is reported in Ref. (44).

Prior to the self shielding calculation proper, Doppler broadening is applied to the infinite-dilution cross sections of resonant isotopes. However, even though occasionally the transfer cross sections are also self shielded, Doppler broadening is not done for the associated transfer kernel of heavy isotopes.⁽⁴⁵⁾ This inconsistency has been the object of renewed attention lately^{(46),(47)} and, because of its possible impact in criticality and, especially, in the analysis of voided situations, it could be of importance for precise core calculations.

4.2 Correlation Angle-energy in Elastic Transfers

Another problem with the multigroup form of the transport equation is the artificial increase of the degree of anisotropy of scattering for elastic and level-inelastic transfers into narrow groups. The reason is that the full angle-energy correlation that characterizes this type of transfers translates into a one-to-one relation between the energy of the scattered neutron and the scattering cosine $\mu = \mathbf{\Omega}' \cdot \mathbf{\Omega}$ and, for groups that are narrow with respect to the slowing down range, the range of the transfer function $P^{g' \rightarrow g}(\mu)$ reduces to only a small part of the full range $[-1, 1]$.

As shown in Appendix A, for elastic or level-inelastic scattering off a target at rest the energy after scattering E and the scattering cosine μ are completely correlated:

$$P(E' \rightarrow E, \mu) = 2P(\mu_{COM}) \frac{H(x_{max} - x)H(x - x_{min})}{(x_{max} - x_{min})E'} \delta[\mu - \mu(x)]. \quad (8)$$

Here the density of probability for the scattering cosine in the center-of-mass (COM) reference system $P(\mu_{COM})$ depends on $x = E/E'$ with $x \in [x_{mi}, x_{max}]$, $H(x)$ is Heaviside's function and $\mu(x)$ is a monotonously increasing function of x . Figure 3 illustrates the shape of the transfer kernel for the case of isotropic scattering in the COM.

Thus, scattering from an energy E' to an energy E in the scattering range results in a single value $\mu = \mu(x)$ for the scattering cosine. Consequently, for scattering from a thin group into another thin group in its scattering range, one obtains a narrow angular range $[\mu_{min}, \mu_{max}] \in [-1, 1]$ for the scattering cosine around the value $\mu(x)$ corresponding to the group averaged energies. Clearly, the expansion in Legendre polynomials of a function such as $P^{g' \rightarrow g}(\mu)$, which vanishes in part of the interval $[-1, 1]$, may require a large number of polynomials and therefore will result in a high degree of anisotropy of scattering. The shapes of the

Fig. 3. Shape of the Transfer Density of Probability $P(E' \rightarrow E, \mu)$ for Level-inelastic Isotropic Scattering in the COM. For Elastic Scattering one Would have $E_{max} = E'$ and $E_{min} = \alpha E'$. For Anisotropic Scattering in the COM the Slowing Down Range and the Area under the Curve will be Preserved, but the Term $P(\mu_{COM})$ will Modify the Straight Shape. However, the Dependence of $\mu(x)$ on the Arrival Energy $E = xE'$ is Not Affected by the Anisotropy of Scattering in the COM.

Fig. 4. $\sigma_s^{g' \rightarrow g}(\mu)$ for Hydrogen in Groups of Unit Lethargy Width Versus μ_c in $[0, 1]$ (Left) and for Oxygen in Groups of 0.04 Lethargy Width Versus μ_c in $[-1, 1]$ (Right). Colors Alternate and Each New Color Corresponds to a New Receiving Group.

multigroup transfer kernels are shown in Fig. 4 for Hydrogen in groups of unit lethargy width and for Oxygen in groups of 0.04 lethargy width, and in Fig. 5 for Sodium and Hydrogen from group 80 of the Xmass mesh.⁽⁴⁸⁾

Standard multigroup libraries contain anisotropic transfer matrices up to a relatively low order of anisotropy and spatially-converged infinite lattice PWR assembly calculations seem to require up to P_3 anisotropy of scattering for light elements (water) in order to get Monte Carlo accuracy.⁽⁴⁹⁾ Since there could be a compensation with the approximation introduced for the computation of shelf shielded multigroup cross sections, this observation does not lead to a clear estimation of the actual effect due to the anisotropy induced by elastic scattering. To measure this effect one needs to write a special discrete ordinate code where multigroup scattering matrices are used to mediate scattering between any two discrete ordinates directions.^{(50),(51),(52)} The formulation to compute

Fig. 5. $\sigma_{g' \rightarrow g}(\mu)$ for Hydrogen from Group 80 of Xmass Mesh to all Other Groups Versus μ_c in $[0, 1]$ (Left) and for Sodium from Group 80 of Xmass Mesh to Groups 80 Through 82 (with Lethargy Widths of 0.15, 0.20 and 0.15) Versus μ_c in $[-1, 1]$ (Right). Colors Alternate and Each New Color Corresponds to a New Receiving Group.

these matrices has already been proposed and preliminary tests have been run.^{(53),(54)} Moreover, if this effect is shown to be important for thin groups it would be possible to perform the calculation of the direction-to-direction transfer matrices with a relatively low increase of isotopic data by combining classical PN transfer data for most of the isotopes and new data for isotopes for which the anisotropy effect from elastic scattering is considered important.⁽⁵⁵⁾

5. ANGULAR DISCRETIZATION

The angular discretization is one of the more important and influential aspects of a deterministic transport calculation. Basically, there are two numerical techniques used for the discretization of the angular variable. To discuss these techniques we consider the one-group transport equation

$$(\Omega \cdot \nabla + \Sigma)\psi = q, \quad (9)$$

where

$$q = \mathcal{H}\psi + S \quad (10)$$

is the emission density which contains the within-group scattering source

$$(\mathcal{H}\psi)(\mathbf{r}, \Omega) = \sum_m^{k(m) \leq K} \Sigma_{k(m)}(\mathbf{r}) A_m(\Omega) \phi_m(\mathbf{r}), \quad (11)$$

where K is the degree of anisotropy of scattering.

5.1 PN Projection

In the projective method the transport equation is projected over a set of angular functions. For instance,

the PN method is based on a set of spherical harmonics spanning a subspace invariant by orthogonal transformations,

$$P_N = \{A_m(\Omega), k(m) \leq N\}.$$

However, lately new projections techniques have been introduced that use expansions into partial-range angular functions, such as wavelets.^{(56),(57)}

The unknown of the PN equations are the angular flux moments $\phi_m(\mathbf{r})$ for $k(m) \leq N$ which for 3D problems yields a total number of unknowns of $M = (N + 1)^2$. The PN projection diagonalizes the scattering term while making an approximation, via the truncation in the order N , on the streaming term; hence, the coupling between the equations arises from the streaming term and, for 3D problems, it couples the equation for $\phi_m(\mathbf{r})$ to eight other equations, namely those for the moments $\phi_m(\mathbf{r})$ with $k'(m') = k(m)$ and $l'(m') = l(m) \pm 1$ and those with $k'(m') = k(m) \pm 1$ and $l'(m') = l(m)$ or $l(m) \pm 1$.

5.2 Discrete Ordinates

The discrete ordinates approximation, also known as the SN approximation, is the most popular way to construct numerical solutions for the one-group transport equation. Basically, this is a collocation technique in the angular variable, whereby the transport equation is solved for a finite set of directions while a set of quadrature weights associated to these directions enables to write the scattering source in terms of the angular fluxes in the prescribed directions. This procedure yields a system of equations for the angular fluxes in the selected angular directions, which are then discretized in the spatial variable. Most of the numerical solutions that are derived from the discrete ordinates equations are plagued with a number of problems such as numerical dispersion and, the behemoth of them all, the so-called ray effect. In spite of this fact, discrete-ordinates-based numerical approximations of the transport equation have an enormous appeal because they lead in a natural way to stable iterative solutions based on source iterations.

To obtain the discrete ordinates approximation of the one-group transport equation we introduce an angular quadrature formula (AQF),

$$S_N = \{w_d, \Omega_d, d = 1, \dots, M\},$$

such that an integral over the angular variable can be approximately evaluated as

$$\int d\Omega' f(\Omega') \sim \sum_d w_d f(\Omega_d).$$

We then write the transport equation for each of the directions in the AQF,

$$(\Omega \cdot \nabla + \Sigma)\psi = q, \quad \Omega \in S_N, \quad (12)$$

and close this system of equations by using the AQF to compute the angular flux moments in terms of the discrete

angular fluxes $\psi_d(\mathbf{r}) = \psi(\mathbf{r}, \mathbf{\Omega}_d)$:

$$\phi_m(\mathbf{r}) = \int d\mathbf{\Omega}' A_m(\mathbf{\Omega}') \psi(\mathbf{r}, \mathbf{\Omega}') \sim \sum_d w_d A_m(\mathbf{\Omega}_d) \psi_d(\mathbf{r}). \quad (13)$$

The discrete ordinates approximation is defined by the set of equations (12) and (13), and, therefore, it is fully specified by the AQF. It consists of a system of coupled PDEs with unknowns the M angular fluxes $\psi_d(\mathbf{r})$. Contrarily to the PN discretization, the SN discretization diagonalizes the streaming term and the equations are coupled via scattering. The solution proceeds by source iterations where at each iteration a sweep over all angular directions is made to obtain a stable solution of a propagation problem with fixed sources.

5.2.1 Angular Quadrature Formulas

As we have seen the basic ingredient of the SN approximation is the AQF and it is not surprising that there has been a sizable number of papers introducing angular quadrature formulas. Stability requires the weights to be positive. Also, in order to preserve reciprocity, the AQF should contain both $\mathbf{\Omega}_d$ and $-\mathbf{\Omega}_d$ with the same weight, a constraint that is enforced in most of the AQFs, although it may be relaxed in direction splitting schemes, where the quadrature formula can be changed from one spatial domain into the next, or for biased formulas in problems with highly forward-peaked scattering.

Because the angular flux can be formally expanded into spherical harmonics, the directions and weights of the angular quadrature should be built so as to exactly integrate a maximum number of products of two spherical harmonics or, equivalently, to integrate a maximum number of spherical harmonics, but symmetry reasons can also be invoked in the construction of the AQF, and most often these formulas are computed by planar symmetries from the directions and weights in the first octant.

For instance, the angular directions of the familiar level-symmetric quadrature are defined so as to preserve not only planar symmetries but also rotations between the axes, while the weights are constructed on the basis of the exact quadrature of spherical harmonics. A problem with this approach is that negative weights result from relatively low orders of the AQF. Negative weights can be avoided by using a product quadrature (PQ) which combines two one-dimensional quadratures with positive weights; typically, a Gauss-Legendre quadrature for the cosine $\mu = \cos\theta$ of the polar angle and a Chebyshev uniform quadrature for the azimuthal angle φ . A disadvantage of the PQ is that, for increasing values of the polar cosine, the quadrature directions concentrate around the polar axis and, as a consequence, the quadrature ‘wastes’ directions. However, because of its precision and ability to integrate spherical harmonics, the PQ is an excellent quadrature. Moreover, the possibility to tailor PQ formulas to specific planar symmetries makes this quadrature an excellent

choice for the exact treatment of geometric boundary conditions and, in particular, for cycling tracking with the method of long characteristics.⁽⁵⁸⁾

Galerkin angular quadratures have been introduced in order to maximize the number of spherical harmonics that can be exactly integrated.⁽⁴³⁾ Here one replaces the angular quadrature set by a ‘directions-to-moments’ Galerkin quadrature matrix M so that formula (13) becomes

$$\phi_m(\mathbf{r}) \sim \sum_d M_{md} \psi_d(\mathbf{r}).$$

Another advantage of this quadrature is that it introduces a collocation-like formulation of the discrete ordinates approximation, which allows for a continuous reconstruction of the angular dependence of the angular flux as a linear combination of angular interpolation polynomials. In principle one can compute a Galerkin matrix from any classical quadrature but the process demands the application of intricate selection rules.⁽⁴³⁾

Finally, Lebedev-type quadratures^{(59),(60),(61)} are constructed so as to be invariant under the action of a finite rotation group and offer the best performance ratio, i.e. the minimal number of directions for a given number of spherical harmonics that are exactly integrated. Moreover, the nodes of these quadratures are nearly uniformly distributed and the associated weights are positive. The rotation groups for the regular polyhedra (platonic solids) have been used to construct bases of interpolation functions and derive Lebedev-type quadratures.⁽⁶²⁾

6. SPATIAL DISCRETIZATION

We consider here numerical techniques for the discretization of the discrete ordinates form of the transport equation, and more precisely two of the most popular techniques: the discontinuous finite element method (DFEM) and the method of long characteristics (MOC).

Most of the methods used for the spatial discretization of the transport equation are based on a partition of the spatial domain into homogeneous regions and a coherent approximation of the flux and the source in each region:

$$\psi(\mathbf{r}, \mathbf{\Omega}) \sim \vec{f}(\mathbf{r}) \cdot \vec{\psi}(\mathbf{\Omega}), \quad (14)$$

where $\vec{f}(\mathbf{r}) = \{f_i(\mathbf{r}), i = 1, P\}$ and $\vec{\psi}(\mathbf{\Omega}) = \{\psi_i(\mathbf{\Omega}), i = 1, P\}$ are the expansion functions and the associated flux components, respectively. Because the regions are homogeneous, this region expansion leads, with no further approximations, to a similar expansion for the sources

$$q(\mathbf{r}, \mathbf{\Omega}) \sim \vec{f}(\mathbf{r}) \cdot \vec{q}(\mathbf{\Omega}) = \sum_m A_m(\mathbf{\Omega}) \vec{f}(\mathbf{r}) \cdot \vec{q}_m, \quad (15)$$

where we have implicitly defined $\vec{q}(\mathbf{\Omega}) = \sum_m A_m(\mathbf{\Omega}) \vec{q}_m$ and $\vec{q}_m = \sum_m \vec{\Phi}_m + \vec{q}_m^{ext}$ comprises within-group scattering and an external source $\vec{q}_m^{ext}$, which accounts for fission and

out-of-the group transfers. Also

$$\vec{\Phi}_m = \int_{(4\pi)} d\Omega A_m(\Omega) \vec{\psi}(\Omega) \quad (16)$$

is a vector containing the spatial moments of the m -th angular flux moment.

To enforce conservation the unit function has to be in the approximation subspace generated by the components of $\vec{f}(\mathbf{r})$ and typically the first component $i = 1$ is taken to be constant over the region.

6.1 The Discontinuous Finite Element Method

Traditional formulations of this method are based on a variational approach. Here, we present the finite element method as a Galerkin projection of the transport equation. The geometry domain is decomposed into a partition of homogeneous regions with similar shapes (a triangularization in finite elements). After multiplication of (9) by a weight function $w(\mathbf{r})$ and integration over a region one gets

$$(-\Omega \cdot \nabla w, \psi) + \Sigma(w, \psi) + \langle w, \psi \rangle_{\pm} = (w, q) + \langle w, \psi_{ups} \rangle_{-}, \quad (17)$$

where we have integrated by parts and replaced the flux on the incoming surface of the region with the flux ψ_{ups} from the upstream cell or eventually from the boundary condition. Also in this equation we have introduced volume and surface scalar fluxes

$$(f, g) = \int d\mathbf{r} (fg)(\mathbf{r}), \quad \langle f, g \rangle_{\pm} = \int_{\pm} dS |\Omega \cdot \mathbf{n}| (fg)(\mathbf{r}),$$

where the volume integral is over the volume of the region and the surface integrals over the incoming (−) or outgoing (+) surfaces of the region.

Next, we introduce a region wise polynomial expansion as in (14) with the components of $\vec{f}(\mathbf{r})$ forming a polynomial basis of order P .

Finally, the equations for the discontinuous finite element method (DFEM) are obtained by using the flux and source expansions in (17) and using as weight functions the polynomials used for the flux expansion (Galerkin projection). From (14) and (15) and with the replacement $w \rightarrow \vec{f}(\mathbf{r})$ one gets

$$[\Sigma M - M_1(\Omega) + N_+(\Omega)] \vec{\psi}(\Omega) = M \vec{q}(\Omega) + N_{-,ups}(\Omega) \vec{\psi}_{ups}(\Omega), \quad (18)$$

where

$$M = (\vec{f}, \vec{f}), \quad M_1(\Omega) = \Omega \cdot (\nabla \vec{f}, \vec{f}) \quad (19)$$

and

$$N_{\pm} = \langle \vec{f}, \vec{f} \rangle_{\pm}, \quad N_{-,ups} = \langle \vec{f}, \vec{f}_{ups} \rangle_{-}.$$

Similarly as the well-known diamond difference method, the DFEM equations are solved with a sweep direction per direction. For each direction the sweep starts at the incoming boundary and the regions fluxes are calculated

replacing $\vec{\psi}_{ups}$ first by the incoming fluxes at the boundary and then by the exiting fluxes of the upstream regions. The flux $\vec{\psi}_{ups}(\Omega)$ in each region is obtained by inverting the matrix in the right hand side (RHS) of Eq. (18).

An equivalent form of the DFEM equations can be written by integrating by parts the term $M_1(\Omega)$ and recasting Eqs. (18) as

$$[\Sigma M + M_1^T(\Omega) + N_-(\Omega)] \vec{\psi}(\Omega) = M \vec{q}(\Omega) + \vec{N}_-(\Omega) \vec{\psi}_{ups}(\Omega), \quad (20)$$

where the upper index ‘ T ’ denotes the transpose matrix. The advantage of this form is that the surface integrations are only done over the incoming surface and this facilitates a better treatment of elements with curved surfaces.⁽⁶³⁾

6.2 The Method of Long Characteristics

To gain a better understanding of the method of (long) characteristics it is better to start with a brief discussion of the method of short characteristics. The latter is a projection technique for Cartesian meshes comprising homogeneous regions. Contrarily to the DFEM which is exclusively based on expansion (14) for the region fluxes, in this method one also introduces an independent surface expansion for the fluxes entering (−) and leaving (+) the region boundary $\psi_{\pm}(\mathbf{r}, \Omega) \sim \vec{f}_{\pm}(\mathbf{r}) \cdot \vec{\psi}_{\pm}(\Omega)$, where the $\vec{f}_{\pm}(\mathbf{r})$ contain surface expansion functions. As for the DFEM, a set of equations for the volume fluxes are obtained by projection over the region expansion functions. These equations are similar to Eqs. (17) but with the difference that the surface angular fluxes in the surface terms $\langle, \rangle_{\pm}$ are written in terms of the independent surfaces expansions introduced for the $\psi_{\pm}(\mathbf{r}, \Omega)$. Next, the system of equations is closed by adding a set of transmission equations for the exiting surfaces fluxes which are obtained by projecting the integral transport equation over the surface expansion functions $\vec{f}_{+}(\mathbf{r})$ for the exiting angular modes.⁽²⁵⁾ Finally, by identifying the angular modes entering a region with the exiting modes from upstream regions, one obtains an iterative numerical solution based in a region to region sweep. The essential point of the method is that the integral form of the transport equation is used to derive the region transmission equation which gives the $\psi_{+}(\mathbf{r}, \Omega)$ in terms of the interior sources and the entering $\psi_{-}(\mathbf{r}, \Omega)$. A particularity of this method is that the approximation for the surface angular modes can be done using the same surface modes for all the angular directions. The reason is that in Cartesian meshes the regions surfaces are flat and an angular direction either enters or leaves a given surface.

Likewise, the method of long characteristics is also based on a partition into homogeneous regions, and volume and surface expansions are again applied to obtain an iterative solution based on region balance and transmission equations. The main difference is that the MOC is designed

for use with unstructured meshes, and that now the exiting and entering boundaries of a region often depend on the angular direction. This calls for the introduction of an angle-dependent representation for the $\psi_{\pm}(\mathbf{r}, \Omega)$, i.e., the representation functions must depend on the angular direction: $\vec{f}_{\pm}(\mathbf{r}) \rightarrow \vec{f}_{\pm}(\mathbf{r}, \Omega)$. Moreover, because of the lack of regularity of unstructured meshes, one is brought to use a piecewise expansion for the surface angular flux modes.

The equations of the method are then defined by a region wise expansion for the angular flux, as in (14), where $\vec{f}(\mathbf{r})$ is a set of spatial functions, typically polynomials, and by an angle-dependent piecewise expansion for the surface exiting and entering modes. To introduce the latter we set $\mathbf{r} = \mathbf{r}_{\perp} + x\Omega$, where $\mathbf{r}_{\perp}$ is a two-dimensional coordinate on a plane orthogonal to Ω and x is the coordinate along the trajectory, and write

$$\psi_{\pm}(\mathbf{r}, \Omega) \sim \sum_t w_t \theta_t(\mathbf{r}_{\perp}) \psi_{t,\pm}(\Omega), \quad (21)$$

where the transverse plane has been partitioned into small surfaces of area w_t and $\theta_t(\mathbf{r}_{\perp})$ is the characteristic function of surface t . Note that the angular flux is not expanded over the region surface but over the plane orthogonal to Ω , which is equivalent to an expansion over the region surface of the current $\psi(\mathbf{r}, \Omega) |\Omega \cdot \mathbf{n}|$ carried by the flux.

The familiar version of the MOC is based on a region wise flat flux approximation, also known as the step approximation, where the expansion in (14) is limited to a single constant function and for simplicity in this section we shall consider only this approximation. Therefore we introduce the simplifications

$$\vec{f}(\mathbf{r}) \rightarrow 1, \quad \vec{\psi}(\Omega) \rightarrow \bar{\psi}(\Omega), \quad \vec{q}(\Omega) \rightarrow \bar{q}(\Omega), \quad (22)$$

where the upper bar denotes the region averaged value.

The transmission equation is obtained by replacing expansions (15) and (21) in integral transport equation (6), with $x = 0$ and $x = x_+$ being the entering and exiting positions for the trajectory across a region, and by integrating the result over transverse surface t . Accounting for the simplifications in (22) we obtain

$$\psi_{t,+}(\Omega) = \langle e^{-\Sigma l} \rangle_t \psi_{t,-}(\Omega) + \langle E \rangle_t \bar{q}(\Omega), \quad (23)$$

where $l = l(\mathbf{r}_{\perp})$ is the chord length within the region, $\langle f \rangle = (1/w_t) \int_t dS_{\perp} f(\mathbf{r}_{\perp})$ denotes the average for all chords emanating from transverse area t and

$$E = \int_0^l dx e^{-\Sigma(l-x)} = (1 - e^{-\Sigma l})/\Sigma$$

is the escape probability for a uniform source. In practice these averaged values are replaced by the value corresponding to a single trajectory (which we also denote by t) centered on the transverse area t :

$$\psi_{t,+}(\Omega) = e^{-\Sigma l} \psi_{t,-}(\Omega) + E_t \bar{q}(\Omega), \quad (24)$$

where E_t is the value of the escape probability for trajectory

t . Figure 6 illustrates the transverse area associated to the trajectory and the ‘tube’ generated by this area across a region.

By identifying the entering flux with the flux exiting the upstream region, transmission equation (24) can then be iteratively used along a trajectory from the entering boundary to the exiting one. The boundary conditions are applied to determine the flux entering the domain and what to do when the trajectory leaves the domain.

Once the sweep is done one has to update the sources for the next iteration. This involves the computation of the moments (16) in terms of the updated region flux. With the help of (14) we write

$$\bar{\psi}(\Omega) = V^{-1} \int d\mathbf{r} \psi(\mathbf{r}, \Omega) = V^{-1} \int dS_{\perp} \int_0^l dx \psi(x), \quad (25)$$

where V is the region volume, the integral in $S_{\perp}$ is over the projection of the region on the transverse plane and $\psi(x)$ is the value of the flux along the trajectory. It remains to use the sweep to compute the integral of the flux over the chord length. This can be done using the differential or the integral form of the transport equation but the result is the same. For example, by integrating the differential form in (4) over the chord length we get

$$\psi_{t,+}(\Omega) - \psi_{t,-}(\Omega) + \Sigma l \bar{\psi}(\Omega) = l \bar{q}(\Omega),$$

where $\bar{f}_t = (1/l) \int_0^l dx f(x)$ denotes the average of $f(x)$ over the chord. Using the last equation in (25) yields

$$\bar{\psi}(\Omega) = V^{-1} \int dS_{\perp} [E_t \psi_{t,-}(\Omega) + C_t \bar{q}(\Omega)],$$

where $C_t = (l - E_t) / \Sigma$. Finally, after the sweep this expression for the averaged flux can be used to update the region averaged flux moments

$$\bar{\Phi}_m = \int_{(4\pi)} d\Omega A_m(\Omega) \bar{\psi}(\Omega)$$

that can be used to compute the source for the next iteration.

Clearly the integral over the angles as well as the

Fig. 6. Transverse Area Associated to a Region. A Trajectory Across the Region and the Transverse Area $dS_{\perp}$ Associated to the Trajectory are Also Shown.

transverse integral over $dS_{\perp}$ are numerically computed. The first with the help of the SN angular quadrature formula and the second using the trajectories,

$$\int dS_{\perp} f(\mathbf{r}_{\perp}) \sim \sum_t w_t f(\mathbf{r}_{\perp,t}),$$

where the sum in t is for all trajectories parallel to Ω that intersect the region. We note that conservation requires the volume V in the equations to be numerically computed using the trajectories.

6.2.1 Tracking Techniques

The first step of a MOC calculation is the computation of the trajectory set. In this step, which depends only on the computing mesh and on the domain boundary conditions but it is otherwise independent of the energy group, a set of parallel trajectories are computed for every angular direction in the SN quadrature set. The minimum information for a trajectory is its direction and transverse weight, Ω and w_t , and a description of its intersections with the regions in the domain: $t = \{r_i, l_i, i = 1, N\}$, where r_i is the order number of the i -th region intersected and l_i the chord length across the region. The set of trajectories can then be used to perform a MOC sweep in any group by just replacing the chord lengths by the corresponding optical distances $l_i \rightarrow \tau_i = \Sigma_i l_i$ and using this group-dependent values to run the proper MOC calculation. The latter is the iterative calculation, region after region, of the exiting flux and the inner fluxes in terms of the incoming flux and the internal sources and, at each region crossing, it relies on coefficients and matrices that depend solely on Σ_i , l_i and $\tau_i = \Sigma_i l_i$. As the transport calculation progress through several outer and many inner iterations, the one-chord calculations are repeated many times and it is therefore essential to optimize the set of operations concerning the treatment of one chord crossing. An example of such optimization can be found in Appendix B for the typical step MOC approximation.

The precision of the MOC calculation is affected by the method that is used to trace trajectories within the domain and the method used to treat reentering boundary conditions. We shall discuss these two points separately.

Trajectories

The problem here is one of optimization, i.e., how to trace trajectories to achieve the best precision while minimizing the number of trajectories? This problem is common to the MOC^{(58),(64)} and the collision probability method and has been previously investigated for the latter⁽⁶⁵⁾ and recently re visited for the MOC.⁽⁶⁶⁾ The main constraint is that the domain contains several regions and that, to avoid a large number of independent trajectories while ensuring numerical conservation along each trajectory, one has to use the same set of trajectories to simultaneously compute the interactions between any two regions in the domain. However, for fixed Ω the value $f_{ij}(\mathbf{r}_{\perp})$ of the interaction between two region i and j depends only on the position $\mathbf{r}_{\perp}$ at which the trajectory intersects the transverse plane, and the function $f_{ij}(\mathbf{r}_{\perp})$ is different from zero only over the intersection $\theta_{ij}(\mathbf{r}_{\perp})$ of the projections of the two regions over the transverse plane. To summarize, one has to introduce a quadrature formula on the entire projection of the domain $\theta(\mathbf{r}_{\perp})$ over the transverse plane which integrates at best the set of functions $\{f_{ij}(\mathbf{r}_{\perp}), \forall i, j\}$, each of which vanish outside a reduced domain $\theta_{ij}(\mathbf{r}_{\perp}) \subset \theta(\mathbf{r}_{\perp})$. This quadrature is defined by a set of weights and coordinates $\{w_t, \mathbf{r}_{\perp,t}, t = 1, N\}$ which are, respectively, the areas associated to the trajectories and the intersection of the trajectories with the transverse plane.

The familiar implementation of tracking is based on the use of a constant step quadrature formula, which corresponds to a set of trajectories evenly spaced on the transverse plane so that their associated areas are equal. An example for the 2D case is illustrated by example I in the left of Fig. 7. The figure shows that the ‘tube’ associated to trajectory t intersects regions 1, 3 and 4. However, the contributions to regions 1 and 4 are zero because the

Fig. 7. Three Different Techniques for Trajectory Tracing. **I:** With Equidistant Tracking the Entire Weight is Assigned to the Regions Intersected by the Trajectory Resulting in Region Numerical Dispersion (RND). **II:** The Projection of Discontinuities Completely Eliminates RND but May Result in too Many Trajectories and Introduces Interface Numerical Dispersion (IND) between Subdomains Independently Tracked. **III:** The Macro Band Technique Eliminates RND from the Interior of the Bands but Introduces IND between Subdomains.

trajectory does not ‘see’ them, while the contribution to region 3 is accounted with the full weight Δ when it should be with weight $\tilde{\Delta}$. A technique to avoid this artificial *region numerical dispersion* (RND) is to project all discontinuities on the transverse plane and to use a higher-order quadrature (Gauss-Legendre for 2D) on each one of the areas so defined to track a set of trajectories emanating from the area. This technique is illustrated in example II in the center of the figure. This quadrature technique is the most accurate and completely eliminates RND. However, as pointed out earlier,⁽⁵⁸⁾ a problem with this method is that the segments generated by the projection of the discontinuities can be very small and very numerous, requiring many trajectories very close to each other. This ‘overkill’ of the technique happens when there are many regions, and therefore discontinuities, in the domain. This is the reason why the technique has been implemented only at the cell level.^{(8),(67),(68),(69)} But a new problem arises here because the projection of discontinuities in neighboring cells do not permit to trace straight trajectories across cell interfaces and this requires an interpolation of the fluxes exiting a cell in order to obtain those entering the neighboring downstream cells. This results on *interface numerical dispersion* (IND) at the cells interfaces. The macro band tracking technique offers a compromise by effectively reducing the number of trajectories while partially suppressing the RND effect.⁽⁷⁰⁾ This is achieved by dividing the transverse area into relatively large subareas, known as macro bands in the 2D case. The ‘tube’ generated by a macro band is divided into segments, which are defined so that the end and beginning of a segment corresponds with the intersection of the ‘tube’ with a single region, and a local projection of discontinuities is then done in the interior of each segment. This technique is illustrated by example III in Fig. 7. However, if the macro band tracking is separately done in subdomains it generates IND. But, in spite of introducing IND, effectuating independent tracking in subdomains, such as cells or assemblies, offers the attractive advantage of allowing for subdomain typing⁵ and therefore reducing trajectory storage needs. This last point is paramount for applications of the MOC to 3D geometries and is discussed further in the last part of Appendix B.

Treatment of boundary conditions and construction of cyclic trajectories

The role of boundary conditions is to determine how to initialize the flux entering the domain and how to terminate the trajectory. Typically, the boundary of the domain is divided into small areas where one computes the exiting and entering currents. These areas can be the external faces of the peripheral regions or, to diminish smearing effects, smaller surfaces obtained by subdividing

the boundary faces.

Boundary conditions can be defined by setting the incoming flux to some given value or by means of a geometric motion or by some albedo condition that uses global or local information on the exiting fluxes to determine the entering ones. Albedo conditions involve the use of more than one exiting flux to determine one entering flux and therefore cannot be used to physically extend the trajectory. On the other hand, geometric motions, such as rotations, specular reflection or translations or, for that matter, any boundary condition defining a single entering flux for every exiting one, can be used to continue the trajectory. The result is a compound trajectory⁽⁵⁸⁾ made up of several single trajectories, each one of which corresponds to a crossing of the domain from an entering position $(\mathbf{r}_{in}, \mathbf{\Omega}_{in})$ to an exiting one $(\mathbf{r}_{out}, \mathbf{\Omega}_{out})$. During tracking the geometric motion at the end of a single trajectory is used to compute the next entering position, $\pi_{exit} : (\mathbf{r}_{out}, \mathbf{\Omega}_{out}) \rightarrow (\mathbf{r}_{in}, \mathbf{\Omega}_{in})$, and the tracking continues from the new entering position $\mathbf{r}_{in}$ with the new direction $\mathbf{\Omega}_{in}$. The description of a compound trajectory requires storing the length and the direction of each single trajectory.

Compound trajectories can be avoided if one stores the exiting fluxes and computes the entering fluxes by interpolating on the exiting ones. This approximated treatment of geometric motions not only increases numerical diffusion (smearing) but has also been proven to be a poor approximation,⁽⁵⁸⁾ and it is definitely better to treat exactly the geometric motions and rely on compound trajectories whenever possible.

One can divide the boundary into an *open* component and a *closed* component, not necessarily continuous. The open component is where there is a fixed entering flux or an albedo boundary condition or an approximation (typically by interpolation) of a geometric motion, while the closed component is where the exact geometric motion is used to put the trajectory back into the domain. Typically a trajectory enters and leaves the domain via the open component of the boundary, and compound trajectories are generated when the boundary contains a closed component that causes the trajectory to reenter one or more times until it leaves through the open component.

This tracking technique is not possible when the open component does not exist. In which case we will say that the domain is closed. For *closed* domains one needs a means to determine the entering flux in order to start a trajectory, and this is provided by the so-called cyclic trajectories. These trajectories are periodic meaning that the trajectory enters the domain at some position $(\mathbf{r}_{in}, \mathbf{\Omega}_{in})$ and bounces back from the boundary reentering the domain one or more times until it reenters at exactly the original position $(\mathbf{r}_{in}, \mathbf{\Omega}_{in})$. From then on the trajectory repeats this cycle *at infinitum*. If we denote by L the length of the trajectory during one cycle, i.e., from an entering position until it reaches again the same entering position, then the flux along the trajectory is periodic with period L so that

⁵ A type is defined by a set of sub domains with identical region mesh.

$\psi(x + L) = \psi(x)$. By using this periodic condition in (5) we obtain

$$\psi_- = \frac{\psi_q(L)}{1 - \psi_{bd}(L)},$$

which allows writing the periodic version of (5) as

$$\psi(x) = \psi_{bd}(x)\psi_- + \psi_q(x).$$

In these formulas, $\psi_{bd}(x) = e^{-\pi(x)}$ and $\psi_q(x) = e^{-\pi(x)} \int_0^x dy e^{\pi(y)} q(y)$ are the components of the flux at x from a unit entering flux and from the sources between 0 and x , respectively. The numerical implementation of the algorithm based on cyclic trajectories requires a solution along the compound trajectory where one first sweeps the trajectory to compute and store the integrals, $\psi_{bd}(i)$ and $\psi_q(i)$, of $\psi_{bd}(x)$ and $\psi_q(x)$ over every track, while cumulating the total values so as to obtain ψ_- at the end of the trajectory. The latter, together with the stored values, allows to update the integral of the flux over every region intersected by the trajectory: $l_i \bar{\psi}_i = \psi_{bd}(i)\psi_- + \psi_q(i)$. Care must be taken because the updating may affect different angular directions for the same region but, otherwise, the implementation is straightforward.

The conditions for a trajectory to be cyclic depend on the shape of the domain and on the type of geometric motions used as boundary conditions but, in any case, they result in a constraint on the trajectory direction. The basic ideas are better discussed using elementary group theory. For example, for two dimensional rectangles or hexagons with translation boundary conditions the group of translations G that act on the reference domain to generate an infinite lattice filling the entire space is a two-dimensional group of the form $G = \{\mathbf{e} = n\mathbf{e}_1 + m\mathbf{e}_2, n, m \in \mathbb{Z}\}$. The $\mathbf{e}_1$ and $\mathbf{e}_2$ are called the generators of the group. For a rectangle we have $\mathbf{e}_1 = a\mathbf{e}_x$ and $\mathbf{e}_2 = b\mathbf{e}_y$, where a and b are the lengths of the horizontal and vertical sides of the rectangle and $\mathbf{e}_x$ and $\mathbf{e}_y$ are the Cartesian unit vectors, while for a hexagon $\mathbf{e}_1 = h(\sqrt{3}\mathbf{e}_x + \mathbf{e}_y)/2$ and $\mathbf{e}_2 = h\mathbf{e}_y$, where $h = \sqrt{3}a$ and a is the side of the hexagon.

Obviously, because cyclic trajectories are periodic they have to be invariant under one of the translations in the symmetry group G . Therefore, a trajectory is cyclic if its direction $\boldsymbol{\Omega}$ is parallel to some vector $\mathbf{e} \in G$. For example, the azimuthal angles and the periods for cyclic trajectories are given by the condition

$$\tan \varphi = \frac{mb}{na}, \quad L = \frac{|n|a}{|\cos \varphi|}$$

for a rectangle and

$$\tan \varphi = \frac{2m+n}{\sqrt{3}n}, \quad L = \frac{\sqrt{3}|n|h}{2|\cos \varphi|}$$

for a hexagon, where we have used the fact that the period equals the length of the vector $\mathbf{e}$ and we require n and m to be coprime. An example is illustrated in Fig. 8 for the case of a rectangle.

To stop cyclic tracking is helpful to know how many

Fig. 8. A Rectangular Domain with Translation Boundary Conditions. The Figure shows a Cyclic Trajectory Generated by the Translation $n = 2$ and $m = 3$.

times a cyclic trajectory bounces off the boundaries. With the exception of singular trajectories that cross through one or more vertices of the domain, all other cyclic trajectories bounce off the boundaries $n + m$ times. These correspond to the n elementary translations in direction $\mathbf{e}_1$ and to the m elementary translations in direction $\mathbf{e}_2$. For the case of the rectangle the translations in the $\mathbf{e}_1$ direction result in the crossing of the horizontal side and we conclude that the trajectory bounces off m times from horizontal sides and n times for vertical sides. A similar argument applies to the hexagonal cell. Another important parameter characterizing cyclic trajectories is the distance between parallel cyclic trajectories. Indeed, although a cyclic trajectory does not change under the action of the translations in G of the form $\mathbf{e}' = k\mathbf{e}$, it does change under the action of all other translations in G . It can be shown that the action of G on a cyclic trajectory generates a family of parallel trajectories that are at a constant distance. The orthogonal distance between two neighbor trajectories is given by the formula

$$\Delta_{\perp} = \frac{|\mathbf{e}_1 \times \mathbf{e}_2|}{L} = \frac{A}{L}, \quad (26)$$

where A is the area of the basic domain. Hence

$$\Delta_{\perp}(\text{rectangle}) = \frac{b|\cos \varphi|}{|n|},$$

$$\Delta_{\perp}(\text{hexagon}) = \frac{\sqrt{3}a|\cos \varphi|}{2|n|}.$$

7. TECHNIQUES BASED ON ASSEMBLY HOMOGENIZATION

We discuss here two improved variants of the two-step core calculation which permit to eliminate or correct

the error introduced by the infinite lattice assembly homogenization. Both techniques are based on a few-macrogroup whole-core transport calculation with full or piece wise homogenized assemblies. The first is a dynamic homogenization technique based on on-the-fly homogenizations with incoming currents provided by neighbor assemblies but normalized to core exchanges as computed by a low-order transport or diffusion model. The second technique is a generalization of the multigroup form of the CETE which allows for fine flux reconstruction with the possibility of re-homogenization, accounting thus for the environment of the assembly in the core. Here a set of multigroup-like homogenized equations which preserve reference reaction rates is obtained from what amounts to a finite element (FE) method in the E -variable. In a different context such multigroup-like equations have been proposed earlier,⁽⁷¹⁾ and applied, in particular, to derive error bounds using FE analysis.⁽⁷²⁾

7.1 Dynamic Homogenization

The classical two-step core calculation is based on the homogenization of assemblies or more complicated motifs involving more than one assembly with specular boundary conditions. With the increasing heterogeneity of present reactor cores, this infinite-lattice homogenization model (ILHM) becomes the more and more questionable. Moreover, reactors concepts with large neutron exchanges across the core, such as the High Temperature Reactor (HTR), are not amenable to this simplified homogenization.

These limitations of the ILHM have motivated researchers to look for more sophisticated homogenization techniques where the core solution is used in a coherent way with the homogenization process. As shown in Fig. 9, the basic idea is based on the observation that the core transport flux in an assembly is the solution of a transport problem for the assembly with fixed eigenvalue $\lambda = \lambda_{core}$ and given incoming boundary fluxes $\psi_{in} = (\psi_{in})_{core}$, where the low index 'core' denotes the values resulting from the whole-core transport calculation:

$$\begin{cases} (\mathbf{\Omega} \cdot \nabla + \Sigma)\psi = (\mathcal{H} + \frac{1}{\lambda_{core}}\mathcal{F})\psi, \\ \psi_{in} = (\psi_{in})_{core}. \end{cases} \quad (27)$$

Hence, to avoid the whole-core fine-group transport calculation, one can proceed with a scheme where the assemblies are independently computed with fine-group transport but the eigenvalue and the coarse neutron exchanges between assemblies are computed using a low-order operator with a few macrogroups. This requires an iterative core calculation where the assemblies are re-homogenized with the core eigenvalue and with incoming fluxes obtained from the angular fluxes leaving the neighbors assemblies, but normalized so as to preserve the core exchanges predicted by the low-order core diffusion or transport calculation.⁽⁷³⁾ An advantage of this approach is that there is no need for the approximate

Fig. 9. The Flux in an Assembly is Uniquely Determined by the Core Eigenvalue and the Flux Entering the Assembly.

power reconstruction used with the typical two-steps method because the solution provides the transport fluxes within the assemblies.

Clearly, the same idea can be translated into a scheme where the low-order core solution is a few macrogroup transport calculation with full or piecewise assembly homogenization. The calculation consists of an iterative core calculation, where the n -th iteration starts with the computations of each assembly with fine-group transport, followed by a homogenization to produce cross sections for the full core macrogroup calculation. If the process has not converged, this later calculation can be used in the next iteration for a new computation and homogenization of each one of the assemblies. Each assembly fine-group transport calculation consists in the solution of a transport problem as in (27) with fixed eigenvalue $\lambda = \lambda_{core}^{(n)}$ and fixed incoming angular fluxes

$$\psi_{in}^g(\mathbf{r}, \mathbf{\Omega}) = \psi_{out}^g(\mathbf{r}, \mathbf{\Omega})|_{neighbor}^{(n-1)} \times \frac{J_{in}^G(\mathbf{r})|_{core}^{(n-1)}}{J_{in}^G(\mathbf{r})|_{neighbor}^{(n-1)}}.$$

Since one solves a source transport problem with fission but fixed eigenvalue, the assembly calculations are much faster than the typical infinite-lattice calculations.^{(74),(75),(76)}

A pivotal aspect of this dynamic homogenization technique is the angular representation for the exiting and entering angular fluxes and, in some sense, this method is basically a degraded interface-current approximation. In a first time, dynamic homogenization could be applied with two-dimensional assembly transport calculations and a three dimensional macrogroup core transport calculation to provide an improved two-step core calculation, but there are still some foreseeable problems for applications to burnup core calculations. In any case, a promising aspect of this technique is to provide acceleration for a 3D full core transport calculation.

7.2 Generalized Energy Condensation

Although the detailed core reaction rates from the continuous energy transport equation (CETE) are not

available, in the context of assembly homogenization theory it is possible to obtain accurate ‘reference’ values from Monte Carlo or from fine multigroup transport assembly calculations. With the help of the assembly reaction rates one can proceed to a formal multigroup homogenization and compute equivalent cross sections for a set of coarse groups, with or without spatial smearing. For a typical multigroup formulation the equations defining this homogenization are identical to those that would be used to write the multigroup form of the CETE.

Rahnema and co-workers^{(77),(78)} and Zhu and Forget^{(79),(80)} have proposed recently a generalized multigroup formulation based on a group wise polynomial expansion in the lethargy variable that allows for an approximate reconstruction of the fine-energy solution. These authors have worked with the lethargy variable but, to keep the notation in this paper, we shall discuss the equations in the energy variable.

We present here a derivation of these equations which follows strictly the formal approach that is used to write the multigroup form of the CETE. The generalized energy condensation method (GECM) is based on the expansion

$$\psi(\mathbf{r}, E, \Omega) = \sum_g \frac{1}{\Delta_g} \sum_{i=0}^{i=\infty} \psi^{gi}(\mathbf{r}, \Omega) f_{gi}(E), \quad (28)$$

where Δ_g is the width of group g , the sum in g is over the set of groups and that in i is over a complete set of expansion functions within each group. The functions $f_{gi}(E)$ are zero outside group g and, without loss of generality, we assume that they obey the orthonormalization conditions

$$\int dE f_{gi}(E) f_{g'i'}(E) = \Delta_g \delta_{gg'} \delta_{ii'},$$

which entails that there is a function, which we take to be the $i=0$ function, which is constant in each group: $f_{g0}(E) = 1$.

To obtain the equations for the GECM we project the CETE over each one of the representation functions. We shall use the notation

$$(f_{gi}, f) = \int dE f_{gi}(E) f(E).$$

The equations one obtains are:

$$(\Omega \cdot \nabla + \Sigma^{gi}) \psi^{gi}(\mathbf{r}, \Omega) = \sum_m A_m(\Omega) \sum_{g'} \Sigma_m^{g' \rightarrow gi}(\mathbf{r}) \Phi_m^{g'}(\mathbf{r}) + \frac{1}{4\pi\lambda} \sum_x \chi_x^{gi} \sum_{g'} (\nu \Sigma_f)_x^{g'}(\mathbf{r}) \Phi_m^{g'}(\mathbf{r}), \quad \forall g, i. \quad (29)$$

In these equation $\Phi_m^g = (f_{g0}, \Phi_m)$ and the cross sections are defined so as to preserve the reference reaction rates:

$$\begin{aligned} \sigma^{gi}(\mathbf{r}, \Omega) &= \frac{(f_{gi}, \sigma\psi)}{(f_{gi}, \psi)}, \\ \sigma_m^{g' \rightarrow gi}(\mathbf{r}) &= \frac{(f_{gi}, (f_{g'0}, \sigma_m \Phi_m))}{(f_{g'0}, \Phi_m)}, \\ (\nu \sigma_f)_x^{g'}(\mathbf{r}) &= \frac{(f_{g'0}, (\nu \sigma_f)_x \Phi)}{(f_{g'0}, \Phi)} \end{aligned} \quad (30)$$

and

$$\chi_x^{gi} = (f_{gi}, \chi_x).$$

For $i=0$ the function $f_{g0}(E) = 1$ is the characteristic function of group g and equations (29) yield an independent set of equations that one readily recognizes as the familiar multigroup form of the CETE:

$$(\Omega \cdot \nabla + \Sigma^g) \psi^g(\mathbf{r}, \Omega) = \sum_m A_m(\Omega) \sum_{g'} \Sigma_m^{g' \rightarrow g}(\mathbf{r}) \Phi_m^{g'}(\mathbf{r}) + \frac{1}{4\pi\lambda} \sum_x \chi_x^g \sum_{g'} (\nu \Sigma_f)_x^{g'}(\mathbf{r}) \Phi_m^{g'}(\mathbf{r}), \quad \forall g, \quad (31)$$

where, for clarity, we have suppressed the index $i=0$ and where the cross sections are those in (30) with $(f_{gi}, f) \rightarrow \int_g dE f(E)$ and $\sum_g \chi_x^g = 1$. As discussed earlier (see Section 4), we note that these equations are what one would expect of a multigroup formulation of the transport equation, with the difference that the total cross section Σ^g depends on the angle and that the transfer coefficients $\Sigma_m^{g' \rightarrow g}$ depend on the two indexes of the spherical function and not simply on the first $k(m)$ index. Hence the multigroup form of the CETE is not a transport equation for an isotropic medium. Furthermore, because of the homogenization process, the microscopic cross sections depend on the spatial position, but this does not affect the nature of the equations. With properly defined boundary conditions the multigroup equations have for solution $\psi^g(\mathbf{r}, \Omega) = \int_g dE \psi(\mathbf{r}, \Omega, E)$ with $\Phi_m^g(\mathbf{r}) = \int_g dE \Phi_m(\mathbf{r}, E)$ and the same eigenvalue as the CETE. Thus, the multigroup form of the CETE preserves the reaction rates, the eigenvalue and the integrals over the macrogroups of the transport fluxes.

Note that for $i > 0$ the right-hand-side of Eq. (29) for each pair (g, i) can be computed using the angular moments and the eigenvalue from the solution of the $i=0$ multigroup equations. Therefore, once Eqs. (31) have been solved, the equation for each pair (g, i) for $i > 0$ can be solved independently with very small numerical effort. Finally, once all the $\psi^{gi}(\mathbf{r}, \Omega)$ for $\forall g$ and $\forall i > 0$ have been computed, one can reconstruct the continuous energy flux from expansion (28) and from this flux and the continuous energy cross sections, or the fine-multigroup ones, one can recover the exact reaction rates for any interval of energy.

In practice, only a few functions would be used per group, not necessarily the same functions or the same number of functions, and the reconstruction just discussed gives an approximation of the fine-group flux in the core. What is essential in order to preserve group reaction rates, fluxes and the eigenvalue is to solve Eq. (31) as posed. It is well known that this can be done with the discrete ordinates (SN) angular approximation by just introducing angle-dependent total cross sections and the dependence on index $l(m)$ of the transfer cross sections, a solution that will require a small modification of an SN code and a small modification of the macroscopic library so as to

account for the angle-dependent cross sections. On the other hand, given the loss of medium isotropy in Eq. (31), the PN angular approximation cannot be used to solve this equation. An example of the solution of Eqs. (31) can be found in Ref. (81) for a 1D slab problem.

To avoid the modifications of the SN code and to facilitate the use of a PN code one can introduce an arbitrary cross section (usually weighted with the transport scalar flux) $\bar{\Sigma}^g(\mathbf{r})$ and write⁶

$$\Sigma(\mathbf{r}, E) = \bar{\Sigma}^g(\mathbf{r}) + (\delta^g \Sigma)(\mathbf{r}, E), \quad E \in g,$$

where $(\delta^g \Sigma)(\mathbf{r}, E) = \Sigma(\mathbf{r}, E) - \bar{\Sigma}^g(\mathbf{r})$. Use of this expression leads to

$$(f_{gi}, \Sigma \psi) = \bar{\Sigma}^g(\mathbf{r}) \psi^{gi}(\mathbf{r}, \Omega) + \sum_m A_m(\Omega) (\delta^g \Sigma)_m^{gi}(\mathbf{r}) \Phi_m^g(\mathbf{r}). \quad (32)$$

The second term in the right-hand-side has been obtained by using the complete spherical harmonic expansion $\psi(\mathbf{r}, \Omega, E) = \sum_m A_m(\Omega) \Phi_m(\mathbf{r}, E)$ to calculate $(f_{gi}, (\delta^g \Sigma) \psi)$ and by defining

$$(\delta^g \sigma)_m^{gi}(\mathbf{r}) = \frac{(f_{gi}, (\delta^g \sigma) \Phi_m)}{(f_{gi}, \Phi_m)}.$$

Finally, when replacing (32) into (29) one may move the sum to the RHS of Eq. (29) and view this term as a within group scattering term. Thus, the equation has been cast as a transport equation in an isotropic medium (albeit with the difference than in multidimensional calculations with anisotropic scattering one has to live with the fact that the transfer cross section $\sigma_m^{g' \rightarrow gi}$ is not that for an isotropic medium). Clearly, a numerical SN or PN solution will require a truncature in the sum in (32) and this introduces an approximation in the conservation of the reaction rates and in the value of the eigenvalue obtained from the $i = 0$ multigroup equations.⁽⁷⁸⁾

Equations (29) and the modification of these equations via (32) have been used in two macrogroups for the calculation of slab reactors comprising one or more assemblies that are homogenized in an infinite-lattice model, and the results show an accurate reconstruction of the fine-multigroup flux for the test case with a single reflected assembly and a good reconstruction for the case of a core comprising several assemblies.⁽⁷⁷⁾ In the initial formulation of the method by Rahnema and co-workers, the expansion functions $f_{gi}(E)$ were shifted Legendre polynomials^{(77),(78)}, whereas discrete Legendre orthogonal polynomials were introduced later.^{(79),(80)} The use of discrete expansion functions is a particular case of the general method illustrated here, when one consider the CETE for

a finite set of energies in each group. With truncated expansions, neither of these two approaches ensure to yield an everywhere positive reconstruction, but the use of discrete Legendre orthogonal polynomials seems to be more stable.⁽⁷⁹⁾

The fine-group reconstructed flux has been observed to give a good approximation of the reference core flux and it can be used to consistently recompute new reaction rates that can then be put to use in a new homogenization to obtain an improved core solution. Numerical tests covering 1D slabs and small 2D cases show that this reconstruction can be iterated to yield very accurate results at a relatively small cost.^{(80),(82)}

8. INTERFACE CURRENT AND RESPONSE MATRIX METHODS

The interface current (IC) approximation is a domain partition method suitable for 3D calculations. The method describes a set of subdomains, which typically will be assemblies, that are coupled via interface fluxes. A variant of the method, the response-matrix (RM) method, is based in the classical two-steps methodology for core calculations and proposes a fast, few-group core transport solution based on pre-calculated response matrices. The advantage of the RM is that no homogenization technique is necessary for the calculations of the assembly response matrices.

8.1 Interface Current Method

In the interface current method the core is decomposed into subdomains. For each subdomain we can write equations given the interior and the exiting fluxes, ψ and ψ_+ , in terms of the interior sources and the incoming fluxes, q and ψ_- . Because of the linearity of the transport equation these equations must be of the form

$$\begin{cases} \psi = I\psi_- + Cq, \\ \psi_+ = T\psi_- + Eq, \end{cases} \quad (33)$$

where the linear operators I , C , T and E stand for ‘incoming’, collision, transmission and escape in a purely absorbing problem.

The idea is to use (33) for an iterative transport calculation of the core, where each iteration would consist of using incoming fluxes and volume sources to solve (33) for each subdomain to obtain interior and exiting fluxes, and use the latter as entering fluxes for the downstream subdomains. To this end we introduce subdomain indexes and note $\psi_{\pm}(i)$ the angular fluxes exiting (+) and entering (−) subdomain i and adopt a global numbering for surface modes to write

$$\vec{\psi}_- = A \vec{\psi}_+. \quad (34)$$

At this point we also abandon the continuous description

⁶ A pioneering discussion of this point, as well as a derivation of the multigroup form of the CETE for transport in a one-dimensional slab can be found in the book by Bell and Glasstone.⁽⁴²⁾ Because of the simplified geometry the analysis in this book missed the subtle change in the transfer cross sections, $\alpha_{k(m)}(E) \rightarrow \sigma_m^g(\mathbf{r})$.

and introduce a numerical representation for the interface angular fluxes so that, with (i, k) denoting the global order number for surface flux mode k in subdomain i , $\vec{\psi}_{\pm} = \{\psi_{\pm}(i, k)\}$ are the global vectors containing all surface modes for all the subdomains.

The ‘connection’ matrix A has to account for possible differences in the numerical representation of surface flux modes from one subdomain to its neighbors as well as for vacuum and reentering boundary conditions. Note that $A_{(i, k), (i', k')}$ vanishes except when i' is an immediate neighbor of i or when $i' = i$ is a peripheral subdomain with re-entering boundary conditions in one or more faces. The rows of A for entering modes associated to vacuum boundary conditions have all entries equal to zero. In the particular case when the spatial and angular representations of entering and exiting modes are identical, A reduces to a ‘permutation’ matrix, except for the entering modes associated to vacuum boundary conditions. To enforce conservation the $A_{(i, k), (i', k')}$ must preserve the exiting current associated to every exiting mode but the detailed calculation of the matrix elements depends on the specific spatial and angular representation.

The solution of the IC equations proceeds by a double iteration: the external iterations are used to update the eigenvalue and the fission source, while the inner iterations solve the one-group source problem represented by Eqs. (33) and (34) by iterations on the incoming fluxes. When the subdomains contain an unstructured geometry one has to rely on computational methods based on pre homogenization or use trajectory-based methods such as the collision probability (CPM) method or the method of characteristics (MOC). However, the CPM cannot account for a variable incoming angular flux or for anisotropy of scattering and, to avoid homogenization, one is left with the MOC. An IC technique based on 2D MOC calculations is described in Section 9.2.

A problem with the use of MOC for subdomains is the cost of the inner source iterations per subdomain, especially when the interface angular fluxes are far from convergence. At this point it is worth to discuss the work by Hong and Cho⁽⁸¹⁾ who considered the approach in (33) for a 2D problem and used the MOC to compute the operators in these equations. However, in order to speed up inner iterations the authors decided to cast the MOC in a matrix form and write the first equation in (33) as

$$\psi(\cdot, \Omega) = I(\Omega)\psi_-(\cdot, \Omega) + C_-(\Omega)q(\cdot, \Omega),$$

where Ω is any direction in the angular quadrature set and the dots indicate spatial variables. In the authors’ implementation the incoming angular flux $\psi_-(\cdot, \Omega)$ was assumed to be piecewise uniform over the boundary of the sub-domain. Therefore, in agreement with the general notation in (33), operator $I(\Omega)$ gives the ballistic contribution of an incoming mode in direction Ω to all the downstream volume fluxes, while operator $C_-(\Omega)$ gives the ballistic contribution to the flux from the volume sources along

the trajectories emanating from the same entering area (which is the reason for the lower index ‘-’). The storage of these angular-dependent first collision ‘probabilities’ allows replacing the typical MOC calculations along all the segments in a trajectory band by a simple matrix vector product, speeding up the source iterations. Once the source iterations have converged, the converged values can be used in the second equation of (33) to determine the exiting angular fluxes.

A way to eliminate the source iterations is to reformulate the IC method so the operators account for scattering. Indeed, one can eliminate scattering contributions and write Eqs. (33) in terms of $\psi_{\pm}$ and the fission source $q_f = \mathcal{F}_{\lambda}\psi$. To do this we use the first equation in (33) to compute $\mathcal{H}\psi$ so that $q = \mathcal{H}I_s\psi_{-} + (1 + \mathcal{H}C_s)q_f$, where, with $X_s = (1 + C\mathcal{H})^{-1}$, $I_s = X_sI$ and $C_s = X_sC$. Then, replacing the new expression for q in the two equations in (33) we get

$$\begin{cases} \psi = I_s\psi_{-} + C_sq_f, \\ \psi_{+} = T_s\psi_{-} + E_sq_f \end{cases} \quad (35)$$

with $T_s = T + E\mathcal{H}I_s$ and $E_s = E(1 + \mathcal{H}C_s)$. Note that one can introduce $Y_s = (1 - \mathcal{H}C)^{-1}$ and use the commutation relations $\mathcal{H}X_s = Y_s\mathcal{H}$ and $X_sC = CY_s$ to write $T_s = T + E_s\mathcal{H}I$, $E_s = EY_s$ and $q = Y_s(\mathcal{H}I\psi_{-} + q_f)$.

The formulation in (35) requires to explicitly compute at least matrices I_s and C_s and we think that, if this approach is selected, then it should be done in the way presented here. However, we are not aware of any implementation of this technique.

8.2 Response-matrix Methods

The final stage in the game we have been playing is to incorporate fission in the operators in (35). This eliminates all internal sources and yields an explicit iteration for the surface angular modes. We use the first equation in (35) to obtain $q_f = Y_{\lambda}\mathcal{F}_{\lambda}I_s\psi_{-}$, where

$$Y_{\lambda} = (1 - \mathcal{F}_{\lambda}C_s)^{-1}, \quad (36)$$

and with the help of the new expression for the fission source we can cast (35) into the form

$$\begin{cases} \psi = I_{\lambda}\psi_{-}, \\ \psi_{+} = T_{\lambda}\psi_{-}, \end{cases} \quad (37)$$

where

$$\begin{aligned} I_{\lambda} &= I_s + C_sY_{\lambda}\mathcal{F}_{\lambda}I_s, \\ T_{\lambda} &= T_s + E_sY_{\lambda}\mathcal{F}_{\lambda}I_s. \end{aligned} \quad (38)$$

Also, by defining $X_{\lambda} = (1 - C_s\mathcal{F}_{\lambda})^{-1}$ and using the commutation relation $X_{\lambda}C_s = C_sY_{\lambda}$, these expressions can be written as $I_{\lambda} = X_{\lambda}I_s$ and $T_{\lambda} = T_s + E_s\mathcal{F}_{\lambda}X_{\lambda}I_s$.⁷

⁷ Another approach is to postulate directly (37) and to obtain the expressions for I_{λ} and T_{λ} directly from (33). Here one uses (1) and the first equation in (33) to get $q = \mathcal{H}_{\lambda}\psi$, and proceed as before to obtain (37) from (33) with $q = \mathcal{H}_{\lambda}I_s\psi_{-}$, $I_{\lambda} = (1 - C\mathcal{H}_{\lambda})^{-1}I$ and $T_{\lambda} = T + E\mathcal{H}_{\lambda}I_s$.

At this point we can note that, regardless of the particular detail of the connection matrix, the introduction of a global angular mode ordering allows to write a global expression for the transmission equation

$$\vec{\psi}_- = \hat{T}_\lambda \vec{\psi}_-, \quad (39)$$

where $\hat{T}_\lambda = AT_\lambda$ is the matrix with elements

$$(\hat{T}_\lambda)_{(i,k),(i',k')}^{gg'} = \sum_{k''} A_{(i,k),(i',k'')} T_\lambda(i')_{k''k'}^{gg'}.$$

Note that $\hat{T}_\lambda$ vanish except if i and i' are neighboring subdomains or if $i' = i$ and subdomain i has a reentering boundary condition. Also, because T_λ comprises scattering and fission, all entering modes of a subdomain are connected to the entering modes of each neighboring subdomain along the common interfaces. Hence, the number of operations involved in multiplying a vector by matrix $\hat{T}_\lambda$ is noticeably reduced. However, unlike the interface current method, the coupling in (34) involves all energy groups and is global, i.e., from any entering mode in a given group to every exiting mode in any group if the subdomain has fission.

Because the subdomain matrices T_λ depend on the global eigenvalue the iterative solution of (39) needs a concurrent calculation of the core eigenvalue. Thus, the iterations can be viewed as the process that updates λ and $\vec{\psi}_-$ until convergence. The updating consists of using the transmission matrices $T_{\lambda^{(n-1)}}$ in (39) to obtain a new value for $\vec{\psi}_-^{(n)}$ and then on computing the eigenvalue from global balance.

$$\lambda^{(n)} = \frac{\sum_i F(i)}{\sum_i [A(i) + J_+(i) - J_-(i)]} \Big|_{(\lambda^{(n-1)}, \vec{\psi}_-^{(n)})}. \quad (40)$$

In this expression $F(i)$, $A(i)$ and $J_+(i) - J_-(i)$ are the fission production, absorption and leakage in subdomain i computed with the previous eigenvalue $\lambda^{(n-1)}$ and the updated incoming fluxes $\vec{\psi}_-^{(n)}$. Each one of these terms is obtained by adding the contributions from each entering mode. If X denotes a generic term, then

$$X = \sum_k X_{(i,k)} \psi_- (i, k),$$

where $X_{(i,k)}$ is the contribution to X from a unit angular flux entering domain i with mode k . Note that during iterations there is no need for computing the internal fluxes or reaction rates via the first equation of (37) and that one only needs to have total subdomain fission production and absorption in order to compute the new eigenvalue.

A direct implementation of this technique requires the pre calculation of matrices I_λ and T_λ per subdomain but these matrices have to be parameterized in terms of the eigenvalue. The storage needed for the matrices is

$$N_G^2 \sum_i N_\lambda(i) \times N_S(i) \times [N_S(i) + N_V(i)], \quad (41)$$

where N_G = number of groups, N_λ = number of λ values for tabulation, N_S = number of surface modes, N_V = number of volume modes. The precision of the method depends on the number of groups, the angular flux representation on subdomain interfaces and the technique used to compute matrices I_λ and T_λ , as well as on the precision of the tabulation in terms of the eigenvalue. A crucial parameter is the number of degrees of freedom $dof = N_S(i) \times N_G$ used in the angular flux representation per domain. The reason is that the precision and the cost (storage, computing time) of the calculation increase with the dof .

In the applications mentioned hereafter the computation of the response matrices were done with Monte Carlo. Also a very low number of groups were used.

In the DRM method of HITACHI^{(83),(84),(85)} a expansion in neutron generations is introduced to avoid the parameterization in terms of λ . Indeed, by using a Neumann expansion in (36) the factor $Y_\lambda \mathcal{F}_\lambda$ in the right-hand side of Eqs. (38) can be written as

$$Y_\lambda \mathcal{F}_\lambda I_s = \frac{1}{\lambda} \sum_{n \geq 0} \left(\frac{1}{\lambda} \mathcal{F}_\lambda \mathcal{C}_s \right)^n \mathcal{F}_\lambda I_s.$$

Hence, T_λ can be computed from four elementary matrices T_s , E_s , $\mathcal{F}_\lambda \mathcal{C}_s$ and $\mathcal{F}_\lambda I_s$ (respectively represented by matrices T , L , A and S in the notation of Ref. (85)). These matrices account for scattering and (only for $\mathcal{F}_\lambda \mathcal{C}_s$ and $\mathcal{F}_\lambda I_s$) for one fission generation with $\lambda = 1$, while the entire fission contribution is explicated by the infinite sum over n . Therefore the evaluation of the final response matrices requires the introduction of a truncated sum and the storage of four matrices per subdomain (akin to set $N_\lambda(i) = 2$ in Eq. (41)). The DRM method minimizes storage and eliminates the error introduced by the interpolation in λ , but adds the computational burden of evaluating the response matrices by what may amount to a costly truncation procedure. The method has been applied to 2D multi assembly configurations⁽⁸³⁾ as well as to a 3D multi assembly configurations and to a 3D ABWR core.^{(84),(85)}

The RM method has been also implemented by Farzad and co-workers at Georgia Tech in the code COMET, but these authors have opted for the parameterization of the response matrices in terms of the eigenvalue, which introduces an approximation via the matrix interpolations. The original derivation of the RM equations was done with a variational formulation^{(86),(87)} but was later reformulated in the simpler form given here.^{(88),(13)} The interface angular modes are a factorized product of space, angle and energy functions,

$$f_{\alpha s, m, g}(\mathbf{r}, \Omega, E) = p_{\alpha s}(\mathbf{r}) h_m(\Omega) \chi_g(E).$$

Here each face of the subdomain has been partitioned into surfaces and $\{p_{\alpha s}(\mathbf{r})\}$ is a set of orthogonal polynomials on surface α ; the $\{h_m(\Omega)\}$ is a set of spherical functions on the half unit sphere and $\chi_g(E)$ is the characteristic function of group g . Clearly, the representation functions of lowest order, $p_{\alpha 0}(\mathbf{r}) = 1$ and $h_1(\Omega) = 1$, are constant. In

order to facilitate partial current conservation the functions are taken to be orthogonal according to the natural surface scalar product

$$\begin{aligned} & (f_{\alpha s, m, g}, f'_{\alpha' s', m', g'}) \\ &= \int_{\partial D_i} dS \int_{(2\pi)^\pm} |\Omega \cdot \mathbf{n}| d\Omega (f_{\alpha s, m, g} f'_{\alpha' s', m', g'}) (\mathbf{r}, \Omega, E) \\ &= C_{\alpha s, m, g} \delta_{\alpha s, \alpha' s'} \delta_{m m'} \delta_{g g'}, \end{aligned}$$

where ∂D_i is the surface of subdomain i and $C_{\alpha s, m, g}$ is a normalization constant.⁽¹³⁾ These orthogonality relations factorize into a relation for the spatial modes times a relation for the angular modes. In particular, the relation for the angular modes can be used to construct a base in the half sphere by a Gram-Schmidt technique. The iterative search for the core eigenvalue has been particularly optimized in the COMET code. On one hand, Eq. (39) is viewed as an eigenvalue equation for the interface angular fluxes,

$$\omega \vec{\psi}_- = \hat{T}_\lambda \vec{\psi}_-,$$

where the eigenvalue ω is expected to converge to 1 as the outer iterations converge to the core eigenvalue. Then, at each outer iteration a power iteration is used to converge the above equation to the critical ω value or, similarly, until the shape of $\vec{\psi}_-$ becomes stable. Hence, contrarily to the traditional approach that uses a pair $(\lambda, \vec{\psi}_-)^{(n-1)}$ in the outer fission loop and one simple iteration of (39) to update the $\vec{\psi}_-$ for the next external iteration, the procedure used in COMET does not require the external iteration in $\vec{\psi}_-$. Moreover, even though this approach converges faster, an initialization with lesser surfaces modes is used to get a first accurate estimate of the eigenvalue.⁽¹³⁾ The method has been applied to time dependent transport problems,^{(89),(90)} coupled photon-electron transport,⁽⁹¹⁾ as well as an imbedded local transport solution for core diffusion calculations of pebble bed reactors in cylindrical $r - z$ and $r - \theta$ geometries.^{(92),(93)} In the latter applications the RM method is applied to the external graphite reflector, which contains control rods and cannot be treated with diffusion theory. In the core calculation a supplementary iteration is done between the core and the outer reflector by using the diffusion partial currents exiting the core to solve the RM transport problem in order to evaluate the albedo condition at the interface between the core and the external reflector. COMET has been also extended to 2D $r - \theta$ and hexagonal geometries^{(94),(95)} and has been recently used to calculate 3D whole-core, few macro groups benchmark problems typical of light and heavy water reactor cores; namely, a stylized 3D PWR problem with UO₂ and MOX fuel, a 3D PWR whole core with gadolinium, a stylized 3D BWR whole core and a stylized 3D CANDU whole core.^{(96),(97),(98),(13)} In particular, this latter calculation shows the flexibility of the RM technique to treat complicated geometries. As an example, the comparison

of COMET against MCNP for the PWR core with the same 8-group library gave a difference of 18 pcm in the eigenvalue, while the mean relative difference in the bundle/assembly averaged and fuel pin averaged fission densities were within 0.2%-0.85% and 0.27%-0.87%, respectively. The preparation of the RM library took about 30 hours on a 30-processor cluster but the final COMET 3D core calculation was 450 times faster than the MCNP core calculation. These preliminary results show that the RM technique can account for transport effects.

Thanks to the pre calculation of the library the RM method can perform in very short times whole core calculations with transport accuracy. This makes the RM method a good candidate for fast reactor-cycle analysis comprising many one-point steady-state whole-core calculations. The main problem to be solved is that of the preparation of a library of response-matrices that realistically account for the time evolution of the subdomains environment or, similarly, of the evolution of the interface spectrum with burn up. This is the problem that all methods depending on a pre compiled library face. For the computation of burnup-dependent response matrices what is needed is the material balance at each burnup step. With the exception of the work reported in Refs. (84)-(85), where it seems that the solution was to compute the response matrices with the material balance predicted by lattice assembly calculations, no other studies have been done. Clearly, the most direct approach consists of using the infinite-lattice approximation as a reference burnup model on which compute burnup-dependent response matrices. A more expensive, but more realistic approach, would be to compute a first burnup step of the whole-core using the response matrices obtained from fresh fuel, and then deplete each assembly with the boundary spectrum obtained from this first whole-core calculation.

Summarizing, the main problems that remain to be solved in order to use the RM method for industrial reactor cycle analysis are: how to define the evolving subdomains environment for the construction of the response matrices, which method might be used to account for interface flux spectral variation within macro groups and the optimization of the interface representation functions. Finally, the storage and computer power needed for the compilation of the parameterized library can be significantly larger than those presently required and there might be a need for parallel computation with distributed memory for the final RM core calculation.

9. MOC-BASED METHODS FOR AXIAL CORES

In this section we consider MOC-based methods for the approximate solution of the 3D transport equation

$$(\Omega \cdot \nabla + \Sigma) \psi = q \quad (42)$$

in an axial domain $D = D_{\perp} \times Z$, where $D_{\perp}$ is a two-dimensional (2D) planar domain and $Z = [z_-, z_+]$ is a one-dimensional (1D) domain, and write $\psi = \psi(\mathbf{r}_{\perp}, z, \boldsymbol{\Omega})$ with $\boldsymbol{\Omega} = (\varphi, \mu)$. To construct a spatial mesh we divide the domain into axial layers $D = \cup_k D_k$ with $D_k = D_{\perp} \times Z_k$ and define a region partition from the tensor product of a layer-dependent 2D mesh on $D_{\perp}$ times a 1D mesh over Z_k . A schematic picture of an axial core geometry is shown in Fig. 10.

We briefly discuss a transverse nodal approach, an interface-current (IC) technique and a synthesis method. The three methods rely on the solutions of 2D problems that can be done with the MOC. In the first approach the 2D equations are coupled to a system of 1D-like equations, in the IC method the coupling is via interface angular fluxes which are given by escape and transmission coefficients from the sources in the layers. The calculation of correct escape and transmission coefficients requires a 3D integration in each layer and this is a truly 3D method. In the last technique the 2D and 1D-like equations are uncoupled. Among these three methods, only the first, known as the ‘fusion’ method, has been implemented and applied to reactor physics calculations.

Not all the details are given. In particular those for the treatment of the collision term, but it seems to the author that there are no surprises hidden.

9.1 The Transverse Nodal Approach

The idea of nodal techniques is to use transverse integration to reduce the multidimensionality of the problem. The basic approximation of the method is done over the ‘transverse currents’ or, more simply, on the angular flux incoming through the transverse direction. The basic ideas have been laid out by Cho and co-workers,^{(99),(100),(101),(102)} under the name of fusion method, and originally implemented in the CRX code⁽¹⁰³⁾ and later in the CHAPLET-3D^{(104),(105)} and the DeCART^{(12),(106)} codes. The accuracy of the method has been checked against the 3D OECD Benchmark C5G7 MOX^{(99),(102),(107),(106),(108)} and also compared to Monte Carlo reference calculations for small 3D ‘reactors’.⁽¹⁰⁵⁾

Fig. 10. Schematics of an Axial Core Geometry.

We consider an axial domain $D = D_{\perp} \times Z$ and proceed by integrating transport equation (42) over the axial and radial directions. Let $D_{\perp} = \cup_r D_r$ and $Z = \cup_k Z_k$ be two partitions of $D_{\perp}$ and Z and assume also that the cross sections are of the form

$$\Sigma(\mathbf{r}) = \sum_k \theta_k(z) \Sigma_k(\mathbf{r}_{\perp}), \quad (43)$$

where $\theta_k(z)$ is the characteristic function of $Z_k = [z_{k-}, z_{k+}]$.

We use now the technique of transverse integration and apply operators $\int_{Z_k} dz$ and $\int_{D_r} d\mathbf{r}_{\perp}$ to Eq. (42). The result can be cast as

$$(\boldsymbol{\Omega} \cdot \nabla_{\perp} + \Sigma_k) \psi_k = q_k - \mu \psi|_{z_{k-}}^{z_{k+}} \quad (44)$$

and

$$(\mu \partial_z + \Sigma_r) \hat{\psi}_r = \hat{q}_r - \int_{\partial D_r} dl (\boldsymbol{\Omega} \cdot \mathbf{n}) \psi. \quad (45)$$

The integral over ∂D_r is done over the one-dimensional boundary of domain D_r and $\mathbf{n}$ is the external normal to the contour. We have also introduced the fluxes

$$\begin{aligned} \psi_k(\mathbf{r}_{\perp}, \boldsymbol{\Omega}) &= \int_{Z_k} dz \psi, \\ \hat{\psi}_r(z, \boldsymbol{\Omega}) &= \int_{D_r} d\mathbf{r}_{\perp} \psi, \end{aligned} \quad (46)$$

and have used similar definitions for q_k and $\hat{q}_r$. We have also assumed, for the time being, that

$$\Sigma_k(\mathbf{r}_{\perp}) = \sum_r \theta_r(\mathbf{r}_{\perp}) \Sigma_{kr} \quad (47)$$

or, in other words, that Σ is piecewise constant in each of the factor domains $D_r \times Z_k$.

We note that the last source term $\mu \psi|_{z_{k-}}^{z_{k+}}$ in the radial 2D equations is not symmetric in $\mu = \cos \theta$ and that, therefore, the radial equations are to be considered for $\theta \in (0, \pi)$, contrarily to the usual treatment of 2D XY transport where the symmetry with respect to the horizontal plane is assumed.

Finally, to obtain a closed system of equations, it remains to introduce nodal approximations for the coupling terms on the right-hand-side of Eqs. (44) and (45). The simplest idea is to use a piecewise constant approximation:

$$\psi(\mathbf{r}_{\perp}, z_{k\pm}, \boldsymbol{\Omega}) \sim \sum_r \frac{1}{A_r} \theta_r(\mathbf{r}_{\perp}) \hat{\psi}_r(z_{k\pm}, \boldsymbol{\Omega}) \quad (48)$$

and

$$\psi(\mathbf{r}_{\perp}, z, \boldsymbol{\Omega}) \sim \sum_k \frac{1}{\Delta_k} \theta_k(z) \psi_k(\mathbf{r}_{\perp}, \boldsymbol{\Omega}), \quad (49)$$

where A_r and Δ_k are, respectively, the area of D_r and the width of Z_k .

The transverse equations are solved with a full-axial range, $\mu \in [-1, 1]$, but otherwise classical 2D MOC method. Several techniques, including finite differencing, step MOC and SPN, have been applied to the solution of

the 1D axial equations which, because it lacks rotation symmetry around the z axis, is not a typical 1D slab problem and involves full angular fluxes. In order to increase the precision of the calculation each layer can be subdivided into several axial regions; moreover, because bottom and top layer fluxes are needed for coupling term (48) it is better to use a numerical solution which gives edge values such as finite-differencing^{(99),(102)} but linear 1D MOC^{(107),(105)} SPN⁽¹⁰⁸⁾ and even diffusion⁽¹⁰⁵⁾ have been used.

The 2D/1D transport iterations were initially accelerated with a linear angular-dependent acceleration⁽⁹⁹⁾ but later on non linear acceleration techniques based on coarse mesh rebalance (CMR) have been successfully applied to the acceleration of inners and outers iterations. Linearization followed by Fourier analysis was used to compare the merits of the basic CMR and the well-known coarse mesh finite difference (CMFD) acceleration methods^{(109),(110)} and the latter has been extensively applied to the acceleration of the transverse nodal equations.^{(111),(112)} An improved version of CMFD, the partial current-based CMFD (p-CMFD) was also developed and used for acceleration.⁽¹¹³⁾ Several variants of CMFD are reviewed in Appendix C. Also, a more involved coarse mesh, angle-dependant rebalance (CMADR) acceleration technique has been proposed and applied to the MOC in 2D XY geometries.^{(114),(115)}

9.1.1 Reaction Rates

Next, we explore in more detail the approximated equations thus obtained. It seems natural that the integrated flux in $D_r \times Z_k$ should be given by the expressions

$$\int_{Z_k} dz \int_{D_r} d\mathbf{r}_\perp \psi(\mathbf{r}, \Omega) = \int_{D_r} d\mathbf{r}_\perp \psi_k(\mathbf{r}_\perp, \Omega) = \int_{Z_k} dz \hat{\psi}_r(z, \Omega)$$

but this is not evident because of approximations (48) in Eq. (44) and (49) in Eq. (45). To check this fact we compute the total reaction rate in $D_r \times Z_k$, $\tau_{kr} = \Sigma_{kr} \int_{Z_k} dz \int_{D_r} d\mathbf{r}_\perp \psi$, first by integrating radial Eq. (44) over D_r and then by integrating axial Eq. (45) over Z_k . For both equations we obtain

$$\tau_{kr} = q_{kr} - \mu \hat{\psi}_r(z, \Omega) \Big|_{z_{k-}}^{z_{k+}} - \int_{\partial D_r} dl (\Omega \cdot \mathbf{n}) \psi_k(\mathbf{r}_\perp, \Omega). \quad (50)$$

This shows that the reaction rates derived from either one equation are identical, and equal to the sources minus the rates of leakage from the $D_r \times Z_k$ domain, where the latter are obtained with coupling assumptions (48) and (49).

However, in practice we are interested for more detailed information, such as the reaction rates in some subdomain $D_{r'} \times Z_{k'} \subset D_r \times Z_k$. If we repeat the previous operations this time integrating over $D_{r'}$ Eq. (44) and over $Z_{k'}$ Eq. (45) we get

$$\begin{aligned} \tau_{kr'}(radial) &= \Sigma_{kr'} \int_{D_{r'}} d\mathbf{r}_\perp \psi_k \\ &= q_{kr'} - \frac{A_{r'}}{A_r} \mu \hat{\psi}_r(z, \Omega) \Big|_{z_{k-}}^{z_{k+}} - \int_{\partial D_{r'}} dl (\Omega \cdot \mathbf{n}) \psi_k(\mathbf{r}_\perp, \Omega) \end{aligned}$$

and

$$\begin{aligned} \tau_{kr'}(axial) &= \Sigma_{kr'} \int_{Z_{k'}} dz \hat{\psi}_r \\ &= q_{kr'} - \mu \hat{\psi}_r(z, \Omega) \Big|_{z_{k'-}}^{z_{k'+}} - \frac{\Delta_{k'}}{\Delta_k} \int_{\partial D_{r'}} dl (\Omega \cdot \mathbf{n}) \psi_k(\mathbf{r}_\perp, \Omega). \end{aligned}$$

Clearly, for $r' \rightarrow r$ and $k' \rightarrow k$ both rates coincide, as proved before. We have also $\sum_{r' \in r} \tau_{kr'} = \sum_{k' \in k} \tau_{kr'} = \tau_{kr}$ so the sum of these reaction rates are conservative for both equations. These reaction rates are conservative when accounting for the leakage terms in their respective equations and can therefore be used. In order to define reaction rates in smaller domains we resort to a technique akin to flux reconstruction and propose:

$$\tau_{kr'} = \frac{\tau_{kr} \tau_{kr'}}{\tau_{kr}}. \quad (51)$$

This formula satisfies $\sum_{r' \in r} \tau_{kr'} = \tau_{kr}$, $\sum_{k' \in k} \tau_{kr'} = \tau_{kr}$ and $\sum_{r' \in r} \sum_{k' \in k} \tau_{kr'} = \tau_{kr}$. If reaction rates are only accessible for the larger domains, then the formula is one of volume proportionality: $\tau_{kr'} = \tau_{kr} (\Delta_{k'} A_{r'}) / (\Delta_k A_r)$.

9.1.2 Cross Section Homogenization

As proposed by Cho and co-workers,^{(99),(102)} it is possible to conjugate the fusion method with cross section homogenization in both radial and axial dimensions. Regarding this we consider that (43) is a good modeling assumption but reexamine now the more offensive assumption (47). If this assumption is not satisfied one has to replace the cross section Σ_r in Eq. (45) by

$$\Sigma_{kr}(\Omega) = \frac{\int_{D_r} d\mathbf{r}_\perp \Sigma \psi}{\int_{D_r} d\mathbf{r}_\perp \psi} \sim \frac{1}{A_r} \frac{\int_{D_r} d\mathbf{r}_\perp \Sigma_k(\mathbf{r}_\perp) \psi_k(\mathbf{r}_\perp, \Omega)}{\hat{\psi}_r(z, \Omega)}, \quad z \in Z_k, \quad (52)$$

where we have introduced an approximation for the numerator. Note that this formula defines an angular-dependent cross section. This dependence can be easily handle in the 1D solution for $\hat{\psi}_r(z, \Omega)$ which, in any case, must be solved for an axial problem which depends on the azimuthal angle φ . A similar approximation has to be introduced in the scattering term contained in q . These cross sections are now angle dependent and Cho and co-workers propose to simplify (52) by replacing $\psi(\mathbf{r}_\perp, \Omega)$ and $\hat{\psi}_r(z, \Omega)$ with the corresponding scalar fluxes. We do not believe, however, that this point is essential to the method. In any case, the cross sections for the axial problems must be computed iteratively. Note that the preceding discussion on reactions rates is also correct at convergence for this case. The interest of homogenization is that it allows to diminish the number of axial equations and/or to allow the radial partitioning $D_\perp = \cup_r D_r$ to change with the axial layer k . Since the solution of the 1D axial systems is much faster than the 2D transverse equations there is, in principle, no need for this homogenization which introduces supplementary approximations in the method.

9.1.3 Higher Spatial Approximations

Closure equations (48) and (49) are based on a solution of the 2D MOC equations by step characteristics. However, for large problems it is suitable to use a higher-order flux expansion and the closure equations can be modified accordingly to include spatial variation along the transverse direction. In this case one may replace (48) with

$$\psi(\mathbf{r}_\perp, z_{k\pm}, \Omega) \sim \sum_r \frac{1}{A_r} \theta_r(\mathbf{r}_\perp) \hat{\psi}_r(z_{k\pm}, \Omega) \times \frac{\tilde{\psi}_{k'}(\mathbf{r}_\perp, \Omega)}{\int_{D_r} d\mathbf{r}_\perp \tilde{\psi}_{k'}(\mathbf{r}_\perp, \Omega)},$$

where $\tilde{\psi}_k(\mathbf{r}_\perp, \Omega)$ is the numerical solution from the 2D problem in layer k' and one may choose $k' = k$ for Ω exiting layer k and k' equal to the neighboring layer for entering directions. In the latter case $\tilde{\psi}_k(\mathbf{r}_\perp, \Omega)$ may be replaced by the incoming flux at an axial boundary. Notice that this closure reduces to (48) for the step approximation and also respects relations (50) for the reaction rates.

9.2 Interface-current Approximation

A problem with any transverse nodal method is that one cannot reconstruct the spatial dependence of the actual multidimensional solution. For the case of the fusion method this means that for $(\mathbf{r}_\perp, z) \in D_r \times Z_k$, one cannot write

$$\psi(\mathbf{r}_\perp, z, \Omega) \sim \psi_k(\mathbf{r}_\perp, \Omega) \times \hat{\psi}_r(z, \Omega)$$

and one has to use an approximate formula for the reaction rate in a 3D subdomain of $D_r \times Z_k$. In order to avoid homogenization and the heuristic reaction rate formula (51) we can connect the different radial layers by interface angular fluxes averaged over the radial domains D_r . Alike the response-matrix method, this technique is also a domain partition with the difference that the local solution depends explicitly in scattering and fission, as in Eq. (33).

The subdomains are the two-dimensional axial layers and the corresponding 3D problem writes as a set of 2D problems connected via interface angular fluxes, as shown in Fig. 11. We solve Eq. (33) by a direct Galerkin-Petrov projection technique over the following expansions for volume and surface fluxes. For the volume fluxes we

Fig. 11. In the Interface-current Method the Layers are Coupled Via Surface Angular Fluxes.

assume

$$\begin{aligned} \psi(\mathbf{r}, \Omega) &\sim \sum_k \theta_k(z) \psi_k(\mathbf{r}, \Omega), \\ \psi_k(\mathbf{r}, \Omega) &\sim \sum_l f_{kl}(z) \psi_{kl}(\mathbf{r}_\perp, \Omega), \end{aligned} \quad (53)$$

where we take the $f_{kl}(z)$ to be orthonormal, $\int_{Z_k} dz f_{kl}(z) f_{kl'}(z) = \delta_{ll'}$.

For the surface angular fluxes we use

$$|\mu| \psi^\pm(\mathbf{r}_\perp, z_{k\pm}, \Omega) \sim \frac{1}{A_r} \sum_r \theta_r(\mathbf{r}_\perp) J_{kr}^\pm(\Omega), \quad (54)$$

where $z_{k\pm}$, $k = 1, 2, \dots$ is the upper boundary of layer k and the $J_{kr}^\pm$ correspond to $\mu > 0$ (+) and $\mu < 0$ (−).

The Galerkin projection over the $\theta_k(z) f_{kl}(z)$ functions gives

$$(\Omega \cdot \nabla_\perp + \Sigma_{kl}) \psi_{kl} = q_{kl} + \mu \sum_{l' \neq l} \alpha_{kl, l'} \psi_{kl'} - \mu f_{kl} \psi|_{z_{k-1}}^{z_k}, \quad \forall k, l. \quad (55)$$

In this expression $\Sigma_{kl} = \Sigma_k - \alpha_{kl}$ and $\alpha_{kl} = \int_{Z_k} dz [\partial_z f_{kl}(z)] f_{kl}(z)$. The result is a set of coupled 2D problems for each layer. If the f_{kl} are polynomials, then the coupling is mild in the sense that the solution can be done iteratively for increasing l order. The surface term in Eq. (55) has to be obtained from numerical approximation (54).

To complete the coupling we need to add the projection over the k interfaces.

For the exiting flux from layer k at z_k we write

$$J_{kr}^+(\Omega) = \int_{D_r} d\mathbf{r}_\perp |\mu| \psi(\mathbf{r}_\perp, z_k, \Omega) = \int_{D_r} dS_\perp \psi(\mathbf{r}_\perp, z_k, \Omega),$$

where the integral in $dS_\perp$ is over the projection of D_r on the surface orthogonal to Ω . Next, we use the integral equation along the back trajectories in layer k to obtain

$$J_{kr}^+(\Omega) = \sum_{r'} T_{k, r r'} J_{k-1, r'}^+(\Omega) + \sum_{l, i} E_{kr} q_{kl i}(\Omega),$$

where i is the region index and where we have assumed that the numerical solution of the 2D problems yield region averaged fluxes and sources, as it is done with the MOC. The computation of the transmission and escape probabilities requires the use of trajectories for each direction Ω . If the solution of the 2D problems is done with the MOC, these trajectories can be obtained by uplifting of the 2D trajectories. Notice also, that all the 2D problems within a layer share the same trajectories and this can be the case also for other layers with the same 2D region layout. The details for the numerical computation of these matrices are not given here but are straightforward.

9.3 Synthesis Techniques

The simplest approach to an approximated 3D solution is to use a synthesis technique. This is also a projection method but this time we use as expansion functions some simpler solutions of the problem. In this case we take

$$\psi(\mathbf{r}, \Omega) \sim \sum_k \hat{\psi}_k(z, \Omega) \psi_k(\mathbf{r}_\perp, \Omega), \quad (56)$$

where the unknown ‘flux’ coefficients are the $\hat{\psi}_k(z, \Omega)$

and the ‘expansion’ functions the $\psi_k(\mathbf{r}_\perp, \mathbf{\Omega})$. The latter are constructed from 2D transport solutions of the type

$$(\mathbf{\Omega} \cdot \nabla_\perp + \Sigma_k) \psi_k = q_k.$$

By inserting the ansatz (56) into the 3D transport equation, using the last equation to eliminate the term $\mathbf{\Omega} \cdot \nabla_\perp \psi_k$ and projecting the result over a set of weights $w_k(\mathbf{r}_\perp, \mathbf{\Omega})$ we get

$$\sum_{k'} [\mu \partial_z \alpha_{kk'}(\mathbf{\Omega}) + \Sigma_{kk'}(z, \mathbf{\Omega})] \hat{\psi}_{k'} = (w_k, q).$$

Here, with the scalar product $(f, g) = \int d\mathbf{r}_\perp (fg)(\mathbf{r}_\perp)$, we have $\alpha_{kk'}(\mathbf{\Omega}) = (w_k, \psi_{k'})$ and $\Sigma_{kk'}(z, \mathbf{\Omega}) = (w_k, (\Sigma - \Sigma_k') \psi_{k'} + q_{k'})$.

The resulting equations form a system of coupled 1D-like transport equations. The Galerkin projection corresponds to the choice $w_k = \psi_k$.

10. CONCLUSIONS

Today there is a number of computer programs able to perform three-dimensional (3D) deterministic transport calculations in a single processor as well as in parallel computers, and some of them have been and are designed to run in massively parallel computers. However, most of the developmental effort is concentrated in achieving high performance in massively parallel machines by increasing the number of groups, angular directions (or spherical harmonics) and number of degrees of freedom (dofs) in the spatial approximation. While this is a laudable goal *per se*, it is important as well to reconsider the physics behind the deterministic approach and also to take into account the industry’s needs and constraints. Deterministic transport methods are based on the discretization of the transport equation in all its variables and among them the most constraining is the multigroup approximation. As we pointed out in this paper, to eliminate or significantly reduce the effects of the self shielding model one needs to use a large number of groups but in turn this results in an increase of the anisotropy of scattering of the transfer matrices. In any case, increasing the number of groups not only results in very large isotopic libraries but it also increases the cost of all the other approximations, because the overall cost of the calculation depends on the total number of inner iterations and each inner concerns the solution of a problem in angle and space. Moreover, although whole-core very precise deterministic transport calculations may be achieved in the future it might be to a high price, requesting expensive machines requiring relatively large power to be run and with high requirement in storage and computing time. These calculations will cover one of the needs of the industry regarding reference calculations and punctual calculations for safety issues, and, more importantly, regarding multiphysics calculations involving neutronics, thermal hydraulics and material models, calculations that massively parallel computers are beginning to make more affordable and precise.

On the other hand, the two-step computing scheme currently used by the industry for core calculations is well fitted for the needs for fast calculations but, because of its reliance on assembly homogenization with two-dimensional (2D) transport calculations and on 3D diffusion core calculations, with the concomitant need for approximate power reconstruction techniques, it needs to be improved. Because of the computing time constraints for reactor cycle analysis involving a large number of whole-core one-point calculations, it does not seem realistic to expect that this goal will be attained by increasing the number of dofs in order to obtain high precision results. In any case, before going this way we need to diminish or, at least, correctly evaluate the errors introduced by other approximations currently used in industrial schemes such as, for example, the length of the time step between calculations or the need for an accurate description of isotopic concentrations. In the meantime it is to be expected that few or relatively few-group 3D transport calculations running in parallel machines with hundreds or a few thousands of processors will make their way in routine reactor analysis calculations. In this paper we have analyzed several transport methods, such as interactive assembly homogenization, response-matrix methods and few-group transport calculations based on the method of characteristics, which show promise for use in the industry in the near future.

Ultimately, any computing method is a compromise between memory requirements and speed of calculation. As we pointed out the cost of a transport calculation is directly linked to the cost of performing a one-group iteration. For methods based on the discrete ordinates form of the transport equation this is the cost involved in doing one sweep, which for the discontinuous finite element method (DFEM) and the method of short characteristics (MOSC) increases with the number of regions and with the number of operations to compute one region. The latter depends on the polynomial degree of approximation used in each region and it has a direct impact in memory storage. For instance, the matrices of the DFEM are a sum of products of quantities that depend only on one variable, such as the multigroup total cross section, the direction cosines or integrals of spatial functions. Therefore these matrices are assembled on the fly and the inverse is also computed on the fly for every calculation of a region. On the contrary, the matrices of the MOSC are the result of numerically expensive multidimensional integrations involving exponentials and the inverse of the system is therefore stored. Because these matrices depend on the energy and on the angular direction, storage requirements may be large. Regarding the popular method of (long) characteristics (MOC) with the step approximation, the situation is better in that the operations to cross a chord over one region are few and need the evaluation of one exponential function which is often obtained from tabulated values. However, the problem now is that several trajectories cross every region and that the cost to treat

one region must be multiplied by the averaged number of trajectories crossing one region. And this number may be on the order of 10 to 20 times more than in the 2D case. There is then a cost involved in going from 2D to 3D. On the other hand, because of the increase in the number of regions, the number of trajectories increases also with the passage to three-dimensions and this may overcome the storage capacity. Thus, contrarily to the DFEM which (in particular thanks to the existence of excellent mesh generators) can make the transition 2D $\rightarrow$ 3D with a minimum of difficulties, the MOC needs rethinking regarding its storage needs as well as the increase in number of operations per region. At least for axial cores, a possibility for reducing the storage for the trajectories is to reconstruct the trajectories from their 2D projections and a small amount of axial-dependent data,⁽¹¹⁶⁾ another possibility illustrated in Appendix B is to use subdomain typing and reconstruct the trajectories from those for the typed subdomains. Furthermore, a decrease in the number of regions can be brought about by the use of high-order approximations. The details have been elaborated in Appendix B.

Finally, there is the ever going ‘antagonism’ between deterministic methods and the ‘embarrassingly’ parallel Monte Carlo method. In spite of our discussion on the physical approximations of deterministic methods in Sections 4 through 6, we believe that with a large enough increase in storage and computing power, deterministic methods with high precision could be run in future massively parallel computers. On the other hand, the memory requirements and the running time of a Monte Carlo 3D whole-core calculation will also be large because of the increase on the number of ‘detectors’ (the equivalent of regions) and, as it is well-known, the fact that the precision of the results increases very slowly with the number of histories and, therefore, with the overall computing time. It might be that the winner would be a combination of the two approaches such as a Monte Carlo calculation with a healthy dose of acceleration provided by 3D whole-core deterministic methods.

Appendix A: Slowing down kernel for a target at rest with isotropic scattering in the COM

We consider elastic or level-inelastic scattering off a target at rest of relative mass $A = M/m$. At low neutron incident energies only elastic scattering is available but, as the energy increases, new inelastic channels will open for the reaction. Hence, the probability $p_k(E')$ for the reaction to exit via channel k is zero for neutron energies E' below the threshold E_k for excitation of the k -th nuclear level and, by denoting with $k = 0$ elastic scattering, we can write

$$\sum_{k \geq 0} p_k(E') = 1.$$

Therefore the scattering kernel is given by

$$P(E' \rightarrow E, \mu) = \sum_{k \geq 0} p_k(E') P_k(E' \rightarrow E, \mu), \quad (57)$$

where

- $\mu = \mathbf{\Omega}' \cdot \mathbf{\Omega}$ = scattering cosine,
- $P_k(E' \rightarrow E, \mu)$ = scattering kernel for channel k .

We consider here an arbitrary exiting channel and denote by Q the initial neutron energy converted into mass of the excited nucleus A^* ($Q = 0$ for elastic scattering). Then, conservation of energy and momenta in the LAB frame gives

$$E' = E + Q + \frac{1}{2} M_\gamma V^2,$$

$$m\mathbf{v}' = m\mathbf{v} + M_\gamma \mathbf{V},$$

where the primes denote quantities before the scattering, $\mathbf{V}$ is the velocity of the nucleus after scattering and

- $M_\gamma = M + Q/c^2$ = mass of excited target.

By neglecting the excess mass, $M_\gamma \sim M$, we obtain:

$$P(E' \rightarrow E, \mu) = 2P(\mu_{COM}) \frac{H(x_{max} - x)H(x - x_{min})}{(x_{max} - x_{min})E'} \delta[\mu - \mu(x)], \quad (58)$$

where for simplicity we have omitted the channel index k ,

- $\mu_{COM} = \mathbf{\Omega}' \cdot \mathbf{\Omega}_{COM}$ = scattering cosine in the COM,
- $P(\mu_{COM})$ = density of probability for μ_{COM} , $\int_{-1}^1 d\mu_{COM} = 1$,
- $\alpha = [(A - 1)/(A + 1)]^2$,
- $x = E/E' \in [x_{min}, x_{max}]$,
- $\sqrt{x_{min}} = \sqrt{\alpha} - \delta_x \sqrt{x_{max}} = 1 - \delta_x$,
- $\delta_x = [(1 + \sqrt{\alpha}/2)[-1\sqrt{1-2\gamma/(1+\sqrt{\alpha})}]]$,
- $\gamma = Q/E'$ = fraction of the initial neutron energy added to the target mass,

$$\mu_{COM} = \frac{2}{x_{max} - x_{min}} \left(x - \frac{x_{max} + x_{min}}{2} \right)$$

and

$$\mu(x) = \frac{\sqrt{x} - (1 - \delta)\sqrt{\alpha/x}}{1 - \sqrt{\alpha}}, \quad (59)$$

with

- $\delta = [(1 + \sqrt{\alpha})/(2\sqrt{\alpha})]\gamma$,
- $\mu(x_{min}) = -1$, $\mu[(1 + \delta)\sqrt{\alpha}] = 0$, $\mu(x_{max}) = 1$.

We note that the slowing down range $(x_{max} - x_{min})E'$ decreases with Q , $\partial_Q(x_{max} - x_{min})E' = \partial_\gamma(x_{max} - x_{min}) = -(1 - \sqrt{\alpha})/(\sqrt{1 - 2\gamma/(1 + \sqrt{\alpha})}) < 0$, but since $\partial_\gamma x_{min} < 0$ lower energies will be reached as Q increases.

The kernel in (58) satisfies the normalization $\int_{x_{min}E'}^{x_{max}E'} dE \int_{-1}^1 d\mu P(E' \rightarrow E, \mu) = 1$ and exhibits a total correlation between the energy after scattering and the cosine of the scattering angle. We shall assume that the $p_k(E')$ in (57) are approximately constant in the departure group g' and write $P(E' \rightarrow E, \mu) \sim \sum_{k \geq 0} p_k^{g'} P_k(E' \rightarrow E, \mu)$.

Therefore, it suffices to compute separately the multigroup transfer kernels associated to each exiting channel:

$$P_k^{g' \rightarrow g}(\mu) = \frac{\int_{g'} dE' (\sigma_s \Phi)(E') \int_g dE P_k(E' \rightarrow E, \mu)}{\int_{g'} dE' (\sigma_s \Phi)(E')}. \quad (60)$$

where $g = [E_g, E_{g-1}]$ and $g' = [E_{g'}, E_{g'-1}]$ are the arrival and departure groups, respectively.

Fig. 12. $\mu(x)$ is a Monotonously Increasing Function of x .

Transfer from group g' reaches all groups $g \geq g'$ with

$$x_{g-1,g'} > x_{\min}, \quad x_{g,g'-1} < x_{\max},$$

where

- $x_{g,g'} = E_g/E_{g'}$.

If g is one of these groups, then the slowing down range in g is $[E_{\min}^g, E_{\max}^g]$, with $E_{\min}^g = \max(E_g, x_{\min}E_{g'})$ and $E_{\max}^g = \min(E_{g-1}, x_{\max}E_{g'-1})$, and the scattering cosine is in the interval $-1 \leq \mu(x_{\min}^g) \leq \mu \leq \mu(x_{\max}^g) \leq 1$ with

$$x_{\min}^g = \max(x_{\min}, x_{g,g'-1}), \quad x_{\max}^g = \min(x_{\max}, x_{g-1,g'}). \quad (61)$$

For elastic scattering off Hydrogen at rest we have $A = 1 - \epsilon$, with $\epsilon \ll 1$, and therefore $\alpha \sim (\epsilon/2)^2 > 0$; hence, for Hydrogen $x \in [(\epsilon/2)^2, 1]$ and $\mu \in [-1, 1]$, although the energy interval, $[(\epsilon/2)^2, (\epsilon/2)]$, where $\mu < 0$ is very small compared to the slowing down range, $[(\epsilon/2), 1]$, where $\mu > 0$. Therefore, it is customary to put $\epsilon = 0$ ($\alpha = 0$) and make the approximation:

$$P_{\text{Hydrogen}}(E' \rightarrow E, \mu) \sim \frac{H(1-x)H(x)}{E'} \delta(\mu - \sqrt{x}),$$

having safely assumed isotropic scattering in the COM, $2P(\mu_{\text{COM}}) = 1$.

At the limit of very thin groups, $|g| = E_{g-1} - E_g \rightarrow 0$, where each group may be identified by its energy, $g \sim E_g$ and $g' \sim E_{g'}$, the transfer $g' \rightarrow g$ is non zero if $x_{\min} \leq x_{g,g'} \leq x_{\max}$ and all arriving particles have a unique $\mu = \mu_{\min} = \mu_{\max} = \mu(x_{g,g'})$.

The conclusion is that the thinner the groups, the narrower the interval of variation $[\mu_{\min}, \mu_{\max}]$ of the cosine of scattering, requesting a higher PN expansion. The nature of the singularity at the limit $|g|, |g'| \rightarrow 0$ is given by Eq. (60): at the limit $|g'| \rightarrow 0$ the integrals in g' vanish in (60) and, accounting for (58), we obtain a delta-like behavior that needs an infinite number of terms in the PN expansion:

$$\lim_{|g|, |g'| \rightarrow 0} P^{g' \rightarrow g}(\mu) = H(x_{\max} - x_{g,g'}) H(x_{g,g'} - x_{\min}) \delta[\mu - \mu(x_{g,g'})].$$

Appendix B: MOC

This appendix comprises four parts. In the first we give an example for the implementation of the step characteristics

based on the use of an exponential tabulation. A general formulation for high-order polynomial approximations with the MOC is given in the second part. In the third part we consider a degraded approximation where the region expansion for the angular flux is replaced by a trajectory-dependent low-order polynomial expansion, while the region expansion for the source is kept. Finally, in the last part we discuss a technique to diminish tracking storage based on subdomain typing and on periodic trajectories.

Inner loop optimization

We address here the optimization of the operations concerning the treatment of a chord length for the familiar step approximation. To simplify and minimize operations we define a minimum value for the total cross section so $\Sigma \geq \Sigma_{\min} > 0$ with, for example $\Sigma_{\min} \sim 10^{-20}$. Then, the operations should be

- before sweeping: compute $q_i(\mathbf{\Omega}) = [q_{\text{ext}}(\mathbf{\Omega}) + (\mathcal{H}\psi)(\mathbf{\Omega})]/\Sigma_i$,
- compute $\tau = \Sigma_i l_i$ and obtain from tabulated values $f(\tau) = 1 - e^{-\tau}$,
- compute $\Delta\psi = f(\tau)(q_i - \psi_-)$ and then $\psi_+ = \psi_- + \Delta\psi$,
- cumulate $\Delta_i(\mathbf{\Omega}) = \Delta_i(\mathbf{\Omega}) + w_i \Delta\psi$,
- after sweeping: compute $\psi_i(\mathbf{\Omega}) = q_i(\mathbf{\Omega}) - \Delta_i(\mathbf{\Omega})/(\Sigma_i V_i)$ and use it to update the scattering source.

The calculation of $f(\tau)$ can be done using a linear, constant step (Δ) tabulation. For $\tau = i\Delta + \alpha$ and $0 \leq \alpha < \Delta$ we compute $x = \tau/\Delta$, $i = \min[i_{\max}, \text{INT}(x)]$ and

$$f(\tau) = f(i) + [f(i+1) - f(i)](x - i).$$

If we want to avoid the computation of the minimum and replace $i = \min[i_{\max}, \text{INT}(x)]$ by $i = \text{INT}(x)$ we have to generate a table for the maximum possible τ . We determine this maximum when computing numerical volumes: $l_{i,\max} = \max_{\mathbf{\Omega}, t/\mathbf{\Omega}} l_i(t, \mathbf{\Omega})$. If a chord normalization is done per angle, then one uses the correction $l_{i,\max} = l_{i,\max}(V_{i,\text{exact}}/V_{i,\text{num}})$. Finally, when the cross section library is accessible prior to the proper MOC calculation, we compute per medium $\Sigma_{m,\max} = \max_g \Sigma_m^g$, then $\tau_{\max} = \max_i (l_{i,\max} \Sigma_{m(i),\max})$ and fabricate the tabulation.

High-order flux expansions

We consider here the general MOC equations for a region wise multifunction expansion as in (14) and (15).

The transmission equation is obtained as for the case of the step approximation but with the difference that now the source is given by (15). This implies that Eqs. (23) and (24) are replaced by

$$\psi_{t,+}(\mathbf{\Omega}) = \langle e^{-\Sigma l} \rangle_t \psi_{t,-}(\mathbf{\Omega}) + \int_0^l dx e^{-\Sigma(l-x)} \vec{f}(x) \cdot \vec{q}(\mathbf{\Omega}) \quad (62)$$

and

$$\psi_{t,+}(\mathbf{\Omega}) = e^{-\Sigma l} \psi_{t,-}(\mathbf{\Omega}) + \vec{E}_t \cdot \vec{q}(\mathbf{\Omega}), \quad (63)$$

where $\vec{f}(x) = \vec{f}(\mathbf{r}_+ + x\mathbf{\Omega})$ is the value of $\vec{f}(\mathbf{r})$ along the trajectory and

$$\vec{E}_t = \int_0^l dx e^{-\Sigma(l-x)} \vec{f}(x)$$

contains the escape coefficients associated to the different components of $\vec{f}(\mathbf{r})$.

The updating of the sources involves the computation of the moments (16) in terms of the updated region flux. With the help of (14) we write

$$\vec{\psi}(\Omega) = M^{-1} \int d\mathbf{r} \vec{f}(\mathbf{r}) \psi(\mathbf{r}, \Omega) = M^{-1} \int dS_{\perp} \int_0^l dx \vec{f}(x) \psi(x), \quad (64)$$

where matrix M has been defined in (19). It remains to use the sweep to compute the integral over the chord length and this can be done by using the differential or the integral form of the transport equation. Contrarily to the step approximation, the final algorithm depends on which equation is used. If we utilize the integral form in (6) we obtain

$$\vec{\psi}(\Omega) = M^{-1} \int dS_{\perp} [\vec{I}_t \psi_{t,-}(\Omega) + C_t \vec{q}(\Omega)] \quad (65)$$

where the vector $\vec{I}_t$ and the matrix C_t ,

$$\vec{I}_t = \int_0^l dx e^{-\Sigma x} \vec{f}(x), \quad C_t = \int_0^l dx e^{-\Sigma x} \vec{f}(x) \int_0^x dy e^{\Sigma y} \vec{f}(y), \quad (66)$$

can be computed analytically. The final formula for the region-averaged angular flux moments is

$$\vec{\Phi}_m = M^{-1} \int_{(4\pi)} d\Omega A_m(\Omega) \int dS_{\perp} \vec{I}_t \psi_{t,-}(\Omega) + \sum_{m'} C_{mm'} \vec{q}_{m'}. \quad (67)$$

The first term on the RHS has to be computed by summing over all trajectory contributions, but in the volume term matrices

$$C_{mm'} = M^{-1} \int_{(4\pi)} d\Omega A_m(\Omega) A_{m'}(\Omega) \int dS_{\perp} C_t$$

are independent of the solution and could be stored. However, this is a set of matrices that depends on anisotropy order, region and group. Storage for a large number of groups is unthinkable because this would lead to a very fast increase in sweep computing time with the order of the polynomial expansion.

On the other hand, use of the differential form of the transport equation leads, after replacement of (14) in (3) and projection of the result over $\vec{f}(x)$, to an implicit linear equation for $\vec{\psi}(\Omega)$:

$$[\Sigma M - M_1(\Omega)] \vec{\psi}(\Omega) = M \vec{q}(\Omega) + \int dS_{\perp} [\vec{f}(0) \psi_{t,-}(\Omega) - \vec{f}(l) \psi_{t,+}(\Omega)], \quad (68)$$

where M_1 has been defined in (19). Finally, we compute $\vec{\psi}(\Omega)$ from (68) and replace in (16) to obtain

$$\vec{\Phi}_m = \int_{(4\pi)} d\Omega A_m(\Omega) X^{-1}(\Omega) \int dS_{\perp} [\vec{f}(0) - e^{-\Sigma l} \vec{f}(l)] \psi_{t,-}(\Omega) + \sum_{m'} D_{mm'} \vec{q}_{m'},$$

where use has been made of (63), $X(\Omega) = \Sigma M - M_1(\Omega)$ and

$$D_{mm'} = \int_{(4\pi)} d\Omega A_m(\Omega) A_{m'}(\Omega) X^{-1}(\Omega) [M - \int dS_{\perp} \vec{f}(l) \vec{E}_t].$$

We point out that conservation requires using the trajectories to compute matrices M and $M_1(\Omega)$. In the limiting case of a step approximation either one of the formulation yields the equations presented in Section 6.2.

Low-order trajectory-dependent approximations

A possibility to simplify and diminish the numerical effort involved with the use of polynomial expansions in the MOC is to replace region wise expansion (14) by a low-order *trajectory-dependent* expansion for the angular flux. Along a trajectory t we assume now⁽¹¹⁷⁾

$$\psi(x) \sim \vec{f}_t(x) \cdot \vec{\psi}_t, \quad (69)$$

where $\vec{f}_t(x)$ has a lower order than the volume expansion in (14), for example for $\vec{f}(\mathbf{r})$ parabolic we can use $\vec{f}_t(x)$ linear or constant. The moments are updated using the expression for $\vec{\psi}(\Omega)$ in Eq. (64) with the only difference that $\psi(x)$ is now computed along the trajectory from the assumption (69) with either the integral or the differential transport equations. Hence, $\vec{\psi}_t$ is computed by projecting over $\vec{f}_t(x)$ either integral Eq. (6) or differential Eq. (4). When the dust has settled we find an expression for the $\vec{\Phi}_m$ similar to (67):

$$\vec{\Phi}_m = M^{-1} \int_{(4\pi)} d\Omega A_m(\Omega) \int dS_{\perp} M_t^L \vec{I}_t^L \psi_{t,-}(\Omega) + \sum_{m'} C_{mm'}^L \vec{q}_{m'},$$

where $M_t^L = \int_0^l dx \vec{f}_t(x) \vec{f}_t(x)$ and

$$C_{mm'}^L = \int_{(4\pi)} d\Omega A_m(\Omega) A_{m'}(\Omega) \int dS_{\perp} M_t^L C_t^L.$$

For the approach based on the integral equation one has

$$\vec{I}_t^L = M_t^{-1} \int_0^l dx e^{-\Sigma x} \vec{f}_t(x), \quad C_t^L = M_t^{-1} \int_0^l dx e^{-\Sigma x} \vec{f}_t(x) \int_0^x dy e^{\Sigma y} \vec{f}_t(y)$$

with $M_t = \int_0^l dx \vec{f}_t(x) \vec{f}_t(x)$, while for the approach using the differential equation:

$$\vec{I}_t^L = X_t^{-1} [\vec{f}_t(0) - e^{-\Sigma l} \vec{f}_t(l)], \quad C_t^L = X_t^{-1} \int_0^l dx e^{-\Sigma x} \vec{f}_t(x) \int_0^x dy e^{\Sigma y} \vec{f}_t(y),$$

where $X_t = (\Sigma M_t - M_{t1})^{-1}$ with $M_{t1} = \int_0^l dx (\partial_x \vec{f}_t)(x) \vec{f}_t(x)$.

Conservation

It remains to check if the trajectory-dependent flux expansion in (69) is conservative. To do this we first prove that this approximation is conservative along trajectories. Conservation depends only on the component over a constant function and, certainly, the finite approximation space spanned by the components of $\vec{f}_t(x)$ contains the constant function 1. Projection over this function of the differential form of the transport equation (4) gives trajectory balance

$$\psi_{t,+} - \psi_{t,-} + \Sigma l \bar{\psi}_t = \int_0^l dx q(x), \quad (70)$$

where $\bar{\psi}_t$ is the chord-averaged angular flux and $\psi_{t,+}$ is given by transmission equation (63). Similarly, by projecting the integral form (6) over the unit function we obtain

$$\Sigma l \bar{\psi}_t = (1 - e^{-\Sigma l}) \psi_{t,-} - e^{-\Sigma l} \int_0^l dx e^{\Sigma x} q(x) + \int_0^l dx q(x),$$

where the source contribution $\int_0^l dx e^{-\Sigma x} \int_0^x dy e^{\Sigma y} q(y)$ has been integrated by parts. Furthermore, use of the transmission equation shows that the precedent equation reduces to (70). We have thus proved that, so far as the constant function is part of the approximation space, any trajectory scheme based on the transmission equation and on the projections of either the differential or the integral form of the transport equation satisfies trajectory conservation relation (70) and this regardless of the value of $\psi_{t,-}$ and of the spatial expansion of the source.

It remains to prove then that the global angular moments obtained from this scheme are region wise conservative. We assume again that global expansion (14) contains a constant element. By projecting over this element we have

$$\begin{aligned} \Sigma V \bar{\Phi}_m &= \int_{(4\pi)} d\Omega A_m(\Omega) \int_{S_\perp(\Omega)} dS_\perp \Sigma l \bar{\psi}_t \\ &= - \int_{(4\pi)} d\Omega A_m(\Omega) \int_{S_\perp(\Omega)} dS_\perp (\psi_{t,+} - \psi_{t,-}) + V \bar{q}_m, \end{aligned}$$

where we have used (70) and the global source expansion (15), and where $\bar{\Phi}_m$ and $\bar{q}_m = \Sigma_m \bar{\Phi}_m + \bar{q}_m^{ext}$ are the region averaged angular moments of the flux and the source and the term with $\psi_{t,+} - \psi_{t,-}$ is the m-th angular moment of the region leakage. Because angular and transverse trajectory quadratures are used to compute entering, exiting and chord averaged angular fluxes, global conservation will be satisfied if and only if all angle and space integrals are calculated with these quadratures.

However, even though both the integral and the differential approximations are conservative, they are not equivalent. The complete forms for the trajectory projections are

$$M_t \bar{\psi}_t = \int_0^l dx \bar{f}_t(x) e^{-\Sigma x} [\psi_{t,-} + \int_0^x dy e^{\Sigma y} q(y)] \quad (71)$$

for the method based on the integral equation and

$$\begin{aligned} (\Sigma M_t - M_{t1}) \bar{\psi}_t &= \int_0^l dx \bar{f}_t(x) q(x) \\ &\quad + [\bar{f}_t(0) \psi_{t,-} - \bar{f}_t(l) \psi_{t,+}] \end{aligned} \quad (72)$$

for the method based on the differential equation.

Integration by parts on the RHS of (71) and using transmission equation (63) gives an equation very similar to (72) with the difference that $M_{t1} \bar{\psi}_t = \int_0^l dx (\partial_x \bar{f}_t(x)) [\bar{f}_t(x) \cdot \bar{\psi}_t]$ in the last equation is replaced by the more correct $\int_0^l dx (\partial_x \bar{f}_t(x)) \psi(x)$ contained in (71), where $\psi(x)$ is given by the exact integral equation in (6). The same analysis can be applied to the equations obtained using global flux expansion (14). Here the difference is that the term $\int d\mathbf{r} \Omega \cdot \nabla \bar{f}_t(x) \psi(x)$ in the integral equation is replaced by the

approximate term $\int d\mathbf{r} \Omega \cdot \nabla \bar{f}_t(x) [\bar{f}_t(x) \cdot \bar{\psi}]$ in the differential one.

Tracking in large domains

One of the main problems with the use of the MOC for large domains and, in particular, for 3D full core calculations is the large amount of data generated by direct tracking. A technique to minimize the tracking is to use local tracking in typed subdomains and reconstruct the full trajectories on the fly. This can be done by identifying subdomains with the same region mesh and tracking for each one of the types.

There are basically two approaches. The first consists of discontinuity projection⁽⁵⁸⁾ or any other technique, like macro bands,⁽⁷⁰⁾ that helps to eliminate or palliate intra region smearing and, therefore, to increase tracking precision. With this technique the iterations proceed region to region in the downstream direction. Moreover, because the exiting trajectories from one subdomain do not match those of the downstream subdomain, an interpolation is needed to get the fluxes entering a subdomain from those leaving the upstream subdomain. If the subdomain is an assembly or in general if it contains a large number of regions, then projection of discontinuities results in a very large number of often very close trajectories and the method is not tracking efficient.⁽⁵⁸⁾ But, even for subdomains with a relatively small number of regions, the technique introduces surface smearing from subdomain to subdomain and this increases numerical diffusion which was supposed to be diminished by the projection.

The second technique is to use modular tracking.^{(68),(119)} This technique relies in cyclic trajectories and can produce a local tracking that is uniformly and symmetrically placed along the surfaces of a subdomain so that the exiting locations of a subdomain match the entering locations of the downstream subdomains. The technique has been developed and tested for the calculations of 2D reactor cores and we shall illustrate it here first in the 2D contest and discuss its extension to 3D calculations later.

For simplicity we consider a rectangular subdomain with horizontal and vertical sides of lengths a and b , respectively. The technique is base on cyclic tracking for a lattice generated by specular symmetries of a basic domain. For the case of the rectangle the formulas are those for the translation boundary condition but applied to a basic domain obtained by symmetries of the original one.⁽⁵⁸⁾ The formulas are as in Sec. 6.2.1 with the replacement $a \rightarrow 2a$ and $b \rightarrow 2b$. Consider a cyclic trajectory defined by the pair of coprime integers (m, n) so that its azimuthal angle satisfies $\tan \varphi = mb/(na)$. Assume we want to cover the horizontal side with N_x parallel trajectories with angle φ and the vertical side with N_y parallel trajectories with angle φ , so that $a = N_x \Delta_x$ and $b = N_y \Delta_y$. However, N_x and N_y must obey the relation $\tan \varphi = \Delta_y/\Delta_x$ which results in the constraints

$$N_x = km, \quad N_y = kn$$

Fig. 13. Example of Two Modular Trackings. Trajectories ($n = 1, m = 3$) for $k = 2$ in a Rectangle with $b/a = 2/3$ (Left) and ($n = m = 1$) for $k = 6$ in a Square. Different Colors Corresponds to Different Periodic Trajectories.

Fig. 14. Modular Tracking ($n = 1, m = 2$) for $k = 2$ in a Square. Trajectories with $\tan \varphi = \pm m/n$ (Left) and with $\tan \varphi = \pm n/m$ (Center). The Latter are Obtained by Diagonal Symmetry from the Former. The Trajectories for a Square with Imposed Diagonal Symmetry (Right) are Obtained by Diagonal Symmetry of Any One of the Previous Sets of Trajectories.

for some integer k . Notice that this approach eliminates trajectory smearing between adjacent subdomains. The best way to determine k is to relate it to precision, i.e., to the distance between trajectories. This gives the formula

$$\Delta_{\perp}(k) = \frac{\Delta_{\perp}}{k},$$

where $\Delta_{\perp}$ is the basic transverse tracking in (26). This technique has also been applied to tracking for cores comprising hexagonal assemblies.

The value of k gives the number of periodic trajectories that will be generated. Because specular boundary conditions are equivalent to translation in a basic domain with double size, the number of times that each trajectory bounces from the horizontal and vertical sides is the double of that for the case with translation boundary conditions, i.e. $2m$ and $2n$ times, respectively. Figure 13 illustrates modular tracking for rectangular and square domains. The more general case of a square with $n \neq m$, where both φ and $\pi - \varphi$ have to be considered,⁽⁵⁸⁾ is shown in Fig. 14. On the right part of this figure it is shown how the generated modular mesh can be applied to a square cell with diagonal symmetry, which will be the case of the central assembly of a core with diagonal symmetry.

Modular tracking has been used for on-the-fly reconstruction of trajectories from typed assemblies for 2D PWR core calculations. In this case only a few

Fig. 15. Modular Tracking in an EPR Core with Typed Assemblies (Example on Left) and Explicit Unstructured Representation of Reflector and Core Surrounding Structures Including Vessel.

Fig. 16. Modular Tracking in a 3D Axial Domain with Rectangular Cross Section. Left: Modular Tracking for the Rectangle $b/a = 2/3$ with $n = 1, m = 3$ and $k = 2$. Right: Modular Tracking for the Vertical Rectangle $c/L_{\perp}$ with $n' = 1, m' = 2$ and $k' = 2$, where $L_{\perp}$ = Total Length of the Horizontal Trajectory on the Left Side of the Figure = $2a\sqrt{5}$.

assembly types are tracked and the total trajectory in the core is constructed out of the components of the periodic trajectories of the typed assemblies. As shown in Fig. 15 this technique can be also used in conjunction with a detailed and fully unstructured description of the reflector and external structures around the core.⁽¹¹⁸⁾ The method can easily be extended to cores composed of typed hexagonal assemblies.^{(68),(118)}

The technique for constructing periodic trajectories using typed assemblies for 2D cores can be easily generalized to 3D axial cores. The idea is illustrated in Fig. 16 for the case of an axial 3D subdomain with rectangular cross section. On the left of the figure modular tracking is applied to the horizontal 2D rectangle with $b/a = 2/3$, $n = 1$ and $m = 3$ which correspond to an azimuthal angle $\tan \varphi = 2$ and to a trajectory length $L_{\perp} = 2a\sqrt{5}$. On the right of the figure modular tracking on the axial direction is applied to the rectangle of horizontal side $L_{\perp}$ and vertical side $c = b$ for $n' = 1$ and $m' = 2$. This results on an azimuthal angle with $\tan \theta = 3\sqrt{5}/2$ and a total trajectory length $L = 28a/3$. The trajectory bounces off $2m = 6$ and $2n = 2$ times from the vertical surfaces associated to a and b , respectively, and $2n' = 2$ times from the top and bottom surfaces associated to c . The trajectories so generated can now be moved so as to enter and exit evenly on each face of the 3D tracking subdomain, as shown in Fig. 17.

Fig. 17. Evenly Distributed Entering and Exiting Locations on the 3D Axial Cell with Rectangular Cross Section with $c = b$ and $b/a = 2/3$ for the Periodic Trajectories in Fig. 16. The Total Length of the 3D Trajectory is $L = 28a/3$.

Appendix C: Coarse mesh finite differences diffusion acceleration

The nonlinear CMFD acceleration is constructed by writing balance equations on coarse mesh homogenized nodes. The homogenization can be done in space or energy or in both and results in

$$\sum_{n'} A_{(nn')} J_{n \rightarrow n'} + V_n \Sigma_n \Phi_n = V_n Q_n, \quad (73)$$

where n is the node, the sum in n' is over the sides nn' of the node, $A_{(nn')}$ and $J_{n \rightarrow n'}$ are the area of side nn' and the averaged net current exiting node n via side nn' , V_n , Σ_n , and Φ_n are the volume of the node and the node averaged removal cross section and flux, and Q_n is the node averaged external source comprising out of group transfers and fission. In our notation n' denotes a side of the node which may be associated with a boundary condition, if the side lays on the boundary of the domain, or may be the common side with the neighboring n' node. Also the double index within parenthesis (nn') denotes a symmetric quantity, $f_{(nn')} = f_{(n'n)}$, while the double index $n \rightarrow n'$ indicates an antisymmetric quantity, i.e., $f_{n \rightarrow n'} = -f_{n' \rightarrow n}$. Notice that $J_{n' \rightarrow n} = -J_{n \rightarrow n'}$.

The node properties are obtained via a process of homogenization so that for any reaction r associated to the node we have

$$\Sigma_{r,n} = \int_n dE d\mathbf{r} (\Sigma_r \Phi)(E, \mathbf{r}) / \int_n dE d\mathbf{r} \Phi(E, \mathbf{r}),$$

where the integration in E is over the macrogroup. The integration domains in energy and space may comprise one or more groups and/or one or more regions of the transport calculation.

For one-group transport acceleration there is no energy condensation and

$$Q_n = \int_n d\mathbf{r} d\Omega q(\mathbf{r}, \Omega)$$

is the total external source in the node as obtained from transport. The acceleration consists of the replacement Φ_r

$\rightarrow f_r \times \Phi_n$, $\forall r \in n$, where $f_r = \Phi_r / \Phi_n$ is the shape factor for the transport flux Φ_r in region r and Φ_n is the averaged transport flux in node n .

For the acceleration of fission iterations the source in macrogroup G is

$$Q_n^G = \sum_{G' \neq G} \Sigma_n^{G' \rightarrow G} \Phi_n^{G'} + \frac{1}{\lambda} \sum_x \chi_{n,x}^G F_x,$$

where λ is the eigenvalue, the sum in x is over all the fissile isotopes in the node and $F_x = \Sigma_x^{G'} (v \Sigma_f^{G'})_{n,x} \Phi_n^{G'}$ is the fission integral for isotope x . Here the acceleration provides the new eigenvalue and the new fission sources F_x for the next fission transport iteration.

Closures for CMFD

To make sure that the nonlinear acceleration reproduces transport converged fluxes it is necessary to enforce conservation. For stability reasons, in the CMFD this is usually done by introducing a drift term in the expression for the net currents $J_{n \rightarrow n'}$ in terms of the node averaged fluxes. This can be done in different ways.

a) The classical CMFD⁽¹⁴⁾ is given by the relation

$$J_{n \rightarrow n'} = -d_{(nn')} (\Phi_{n'} - \Phi_n) - s_{n \rightarrow n'} \hat{d}_{(nn')} (\Phi_{n'} + \Phi_n), \quad (74)$$

where $s_{n \rightarrow n'} = 1$ if the spatial variable normal to side nn' increases in direction $n \rightarrow n'$ and $s_{n \rightarrow n'} = -1$ otherwise. Notice that $s_{n \rightarrow n'}$ is an antisymmetric quantity.

In Cartesian meshes

$$d_{(nn')} = \frac{d_n d_{n'}}{d_n + d_{n'}}$$

comes from the usual finite-differences discretization for the interface current, with $d_n = 2D_n/h_{nn'}$ and $h_{nn'}$ denoting the mesh side for node n in direction normal to side nn' , and the artificial drift coefficient

$$\hat{d}_{(nn')} = -s_{n \rightarrow n'} \frac{J_{n \rightarrow n'} + d_{(nn')} (\Phi_{n'} - \Phi_n)}{\Phi_{n'} + \Phi_n} \Big|_{transport}$$

is computed using currents and fluxes from the transport sweep so as to ensure that $\Phi_n = \Phi_n'$ if the transport sweep has converged.

b)p-CMFD ('p' is for 'partial'): Another possibility is to introduce independent corrections on the partial currents^{(113),(109)} by writing $J_{n \rightarrow n'} = J_{n \rightarrow n'}^+ - J_{n' \rightarrow n}^+$ and assuming the relation

$$J_{n \rightarrow n'}^+ = -\frac{1}{2} d_{(nn')} (\Phi_{n'} - \Phi_n) - s_{n \rightarrow n'} \hat{d}_{nn'} \Phi_n$$

and a similar formula for $J_{n' \rightarrow n}^+$. The $\hat{d}_{nn'}$ is obtained by enforcing transport balance in the previous equation:

$$\hat{d}_{nn'} = -s_{n \rightarrow n'} \frac{2J_{n \rightarrow n'}^+ + d_{(nn')} (\Phi_{n'} - \Phi_n)}{2\Phi_n} \Big|_{transport}.$$

The total net current is given by the expression

$$J_{n \rightarrow n'} = -d_{(nn')} (\Phi_{n'} - \Phi_n) - s_{n \rightarrow n'} (\hat{d}_{nn'} \Phi_{n'} + \hat{d}_{nn'} \Phi_n), \quad (75)$$

c)AFC (average flux correction): This model suggested by Yamamoto^{(120),(121)} is also based on two adjustable

coefficients. Here one poses

$$J_{n \rightarrow n'} = -d_n [\Phi_{(nn')} - \Phi_n + s_{n \rightarrow n'} \hat{d}_{nn'} \Phi_n],$$

where $\Phi_{(nn')}$ is the interface flux, and similarly for $J_{n' \rightarrow n}$. The coefficients $\hat{d}_{nn'}$ and $\hat{d}_{n'n}$ are obtained by enforcing transport balance in the expressions for $J_{n \rightarrow n'}$ and $J_{n' \rightarrow n}$:

$$\hat{d}_{nn'} = -s_{n \rightarrow n'} \frac{J_{n \rightarrow n'} + d_n (\Phi_{(nn')} - \Phi_n)}{d_n \Phi_n} \Big|_{transport}.$$

Finally, by computing $d_n J_{n \rightarrow n'} - d_{n'} J_{n' \rightarrow n} = (d_n + d_{n'}) J_{n \rightarrow n'}$ we eliminate the interface flux and obtain a final equation for the current in terms of the region averaged fluxes:

$$J_{n \rightarrow n'} = -d_{(nn')} [\Phi_{n'} - \Phi_n + s_{n \rightarrow n'} (\hat{d}_{nn'} \Phi_n + \hat{d}_{n'n} \Phi_{n'})]. \quad (76)$$

A related technique has been recently suggested where the parameter $d_{(nn')}$ is based on a simplified Eddington factor and a multiplying parameter is introduced to ensure stability.^{(122),(123)}

d) Another somewhat simpler formula (SYW) is to set

$$J_{n \rightarrow n'}^+ = -s_{n \rightarrow n'} \hat{d}_{nn'} \Phi_n$$

and a similar expression for $J_{n' \rightarrow n}^+$. In this case

$$J_{n \rightarrow n'} = -s_{n \rightarrow n'} (\hat{d}_{nn'} \Phi_n + \hat{d}_{n'n} \Phi_{n'}). \quad (77)$$

Therefore there is no physics and everything is obtained from transport balance. Here we have

$$\hat{d}_{nn'} = -s_{n \rightarrow n'} \frac{J_{n \rightarrow n'}^+}{\Phi_n} \Big|_{transport}.$$

This case is equal to the limit of p-CMFD for $d_{(nn')} \rightarrow 0$.

General form

Clearly all these models can be written as

$$J_{n \rightarrow n'} = \alpha_{n'n} \Phi_n - \alpha_{nn'} \Phi_{n'} \quad (78)$$

where for CMFD

$$\alpha_{n'n} = \frac{J_{n \rightarrow n'} + 2d_{(nn')} \Phi_{n'}}{\Phi_{n'} + \Phi_n} \Big|_{transport},$$

$$\alpha_{nn'} = \frac{-J_{n \rightarrow n'} + 2d_{(nn')} \Phi_n}{\Phi_{n'} + \Phi_n} \Big|_{transport},$$

for p-CMFD

$$\alpha_{n'n} = \frac{2J_{n \rightarrow n'}^+ + d_{(nn')} (\Phi_{n'} + \Phi_n)}{2\Phi_n} \Big|_{transport},$$

$$\alpha_{nn'} = \frac{2J_{n' \rightarrow n}^+ + d_{(nn')} (\Phi_{n'} + \Phi_n)}{2\Phi_{n'}} \Big|_{transport},$$

for AFC

$$\alpha_{n'n} = d_{(nn')} \frac{J_{n \rightarrow n'} + d_n \Phi_{(nn')}}{d_n \Phi_n} \Big|_{transport},$$

$$\alpha_{nn'} = d_{(nn')} \frac{-J_{n \rightarrow n'} + d_{n'} \Phi_{(nn')}}{d_{n'} \Phi_{n'}} \Big|_{transport},$$

and for SYW

$$\alpha_{n'n} = \frac{J_{n \rightarrow n'}^+}{\Phi_n} \Big|_{transport},$$

$$\alpha_{nn'} = \frac{J_{n' \rightarrow n}^+}{\Phi_{n'}} \Big|_{transport}.$$

Implementation of boundary conditions

We consider geometric boundary conditions and albedo boundary conditions. For all these conditions it seems better not to respect the currents obtained from transport, especially if the transport sweep iterates also in the boundary condition and, instead, enforce the exact boundary condition for the diffusion acceleration.

For geometric motion we will then use

$$J_{n_{in} \rightarrow n'} = -J_{n_{out} \rightarrow n'},$$

where n_{in} is the incoming boundary node and n_{out} the outgoing one. For specular reflection $n_{in} = n_{out}$, while for translation n_{in} and n_{out} are opposite nodes. For multi dimensional geometries one has to account for the angular direction change for rotations and specular symmetries.

For albedo approximate boundary conditions (vacuum and albedo) the boundary condition reads $J_{n \rightarrow n'}^- = \beta J_{n \rightarrow n'}^+$, where nn' indicates a surface of region n laying on the boundary of the domain. This leads to the relation

$$J_{n \rightarrow n'} = (1 - \beta) J_{n \rightarrow n'}^+.$$

We recognize that our final expression must be as in (78) but with $\alpha_{nn'} = 0$. This equation can be used to compute $\alpha_{n'n} = J_{n \rightarrow n'} / \Phi_n \Big|_{transport}$, but we prefer to use an expression converged on the boundary condition and replace $J_{n \rightarrow n'} / \Phi_n \Big|_{transport}$ with $(1 - \beta) J_{n \rightarrow n'}^+ / \Phi_n \Big|_{transport}$, which leads to

$$\alpha_{nn'} = 0,$$

$$\alpha_{n'n} = (1 - \beta) \frac{J_{n \rightarrow n'}^+}{\Phi_n} \Big|_{transport}.$$

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